This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-96SR18500 with the U. S. Department of Energy.

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**Key Words:** Salt Disposition Crystalline Silicotitanate

### High Level Waste System Impacts from Small Column Ion Exchange Implementation

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August 18, 2005



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## **Summary**

The objective of this task is to identify potential waste streams that could be treated with the Small Column Ion Exchange (SCIX) and perform an initial assessment of the impact of doing so on the High-Level Waste (HLW) system. Design of the SCIX system has been performed as a backup technology for decontamination of High-Level Waste (HLW) at the Savannah River Site (SRS). The SCIX consists of three modules which can be placed in risers inside underground HLW storage tanks. The pump and filter module and the ion exchange module are used to filter and decontaminate the aqueous tank wastes for disposition in Saltstone. The ion exchange module contains Crystalline Silicotitanate (CST in its engineered granular form is referred to as IONSIV® IE-911), and is selective for removal of cesium ions. After the IE-911 is loaded with Cs-137, it is removed and the column is refilled with a fresh batch. The grinder module is used to size-reduce the cesium-loaded IE-911 to make it compatible with the sludge vitrification system in the Defense Waste Processing Facility (DWPF). If installed at the SRS, this SCIX would need to operate within the current constraints of the larger HLW storage, retrieval, treatment, and disposal system. Although the equipment has been physically designed to comply with system requirements, there is also a need to identify which waste streams could be treated, how it could be implemented in the tank farms, and when this system could be incorporated into the HLW flowsheet and planning. This document summarizes a preliminary examination of the tentative HLW retrieval plans, facility schedules, decontamination factor targets, and vitrified waste form compatibility, with recommendations for a more detailed study later. The examination was based upon four batches of salt solution from the currently planned disposition pathway to treatment in the SCIX. Because of differences in capabilities between the SRS baseline and SCIX, these four batches were combined into three batches for a total of about 3.2 million gallons of liquid waste. The chemical and radiological composition of these batches was estimated from the SpaceMan Plus<sup>TM</sup> model using the same data set and assumptions as the baseline plans.

Modeling of the ion exchange performance of the three selected waste batches indicates that 20 columns (375 gallons each) of IE-911 would be needed to reach 0.005 Ci/gal in the effluent, and would require about 21 months of operation. An alternate target of 0.08 Ci/gal could be reached using 15 columns in about 11 months, if the other system components, such as the filter, can support this higher flow rate. In either case, SCIX treatment of the salt solution would reduce the volume of liquid disposed in Saltstone by about 1.9 million gallons, compared to the baseline. Using the lower effluent target of 0.005 Ci/gal, disposal of the Cs-loaded IE-911 in the DWPF vitrified waste form is expected to increase the number of canisters by 19, although there are many assumptions within this projection. Interestingly, mixing IE-911 with a preliminary projected composition of Sludge Batch #4 (SB4) and various frits increased the projected operating windows (which are based on projected waste loadings) based on model predictions. The models associated with the Product Composition Control System (PCCS) predicted that for the baseline SB4 case used, sludge alone could be accommodated at 25–30 wt% total oxides but increases to 25-32 wt% with IE-911, although the higher volume of the mixture still resulted in more canisters. The 2 wt% improvement in loading was consistent for a range of anticipated waste compositions and quantities. Depending on several assumptions of sludge volume and composition, the change in number of projected DWPF canisters ranges from a decrease of 8 canisters to an increase of 19. The current limit for titania in glass (1 wt%) was not exceeded at the maximum 32 wt% oxide loading in the baseline case, although it was so close (0.986 %) that the "measurement uncertainty" in the models required relaxation of the limit.

As with any new stream that is introduced in the HLW system or as with planning for a new sludge batch, the impacts on the HLW system (e.g., Tank Farm, Saltstone, DWPF) need to be evaluated and understood before the initiation of processing of that stream. The incorporation of the SCIX stream is no different. In the case of DWPF, resolution of uncertainties and verification of assumptions are needed before a firm estimate on canister count and other system impacts can be made. Based on a preliminary judgment, the IE-911 option is considered plausible and has the potential to offer advantages from a processing time and waste generation perspective, but various issues regarding the process ability of the feed through the Chemical Processing Cell and melter should be further assessed to adequately quantify the impacts and risks. Finalized implementation plans for both the baseline and SCIX treatment scenarios are needed, along with a SpaceMan Plus<sup>TM</sup> simulation using a SCIX treatment module to confirm that critical infrastructure components are available when needed (e.g. tank space, transfer lines).

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### Acronyms

ARP Actinide Removal Process

Ci Curie

CPC Chemical Process Cell (at DWPF)

CST Crystalline Silicotitanate (powdered sorbent)  $\Delta G_P$  preliminary glass dissolution estimator

DF Dilution Factor (of IONSIV® IE-910 by binder in IE-911)

DWPF Defense Waste Processing Facility

g gram

gpm gallons per minute
HLW High Level Waste
IE-910 IONSIV® IE-910 (CST)

IE-911 IONSIV® IE-911 (granular form of CST)

M Molarity mL milliliter

MAR Measurement Acceptability Region

MCU Modular Caustic Side Solvent Extraction Unit

MFT Melter Feed Tank

MST Monosodium Titanate (Sr and actinide sorbent)

ORNL Oak Ridge National Laboratory
PCCS Product Composition Control System

SB Sludge Batch

SCIX Small Column Ion Exchange

SME Slurry Mix Evaporator

SRAT Sludge Receipt and Adjustment Tank SRNL Savannah River National Laboratory

 $\begin{array}{ll} SRS & Savannah \ River \ Site \\ T_L & liquidus \ temperature \end{array}$ 

VERSE-LC VErsatile Reaction Separation (computer modeling program)

WAC Waste Acceptance Criteria WCS Waste Characterization System

WL waste loading

ZAM (no acronym) computer model of ion exchange equilibrium for CST

η viscosity

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### 1.0 Introduction

### 1.1 Objective and Methodology

The objective of this task is to identify potential waste streams that could be treated with the Small Column Ion Exchange (SCIX) and perform an initial assessment of the impact of doing so on the High-Level Waste (HLW) system. The assessment evaluates the impact on the (a) volume of waste treated, (b) tank farm storage space, (c) Saltstone product volume, and (d) Defense Waste Processing Facility (DWPF).

This evaluation is in support of a task led by Oak Ridge National Laboratory (ORNL). Funding for this alternative project is provided by the Department of Energy EM-21 office.

To accomplish this objective, the tentative waste treatment plans were reviewed to identify a logical implementation plan. The output from a baseline run of the SpaceMan Plus ™ software (a Visual Basic model of the SRS liquid waste and waste solidification system; Elder, et al., 2004) was used to obtain the waste stream compositions in the conceptualized implementation plan. These compositions were then used as inputs to the ZAM and VERSE models (Crystalline Silicotitanate [CST] absorption and column performance models; Zheng and Anthony, 1996, Whitley and Wang, 1998) to determine the quantity of IONSIV® IE-911 needed and to estimate the processing impacts and schedule. The quantity of spent IE-911 generated was then coupled with a projected sludge waste composition and the Product Composition Control System (PCCS) model (glass durability model; Brown, Postles, and Edwards, 2002) was used to evaluate the impact on the projected operating window which ultimately led to an assessment on the impact to DWPF canister production.

### 1.2 SCIX Process Description

The SCIX system is being designed for possible installation in a HLW tank (Walker, et al., 2004). The system consists of three modules that fit inside of risers (replacing the plugs) and three shielded transfer lines on top of the tanks (i.e., feed, product, and loaded ion exchange sorbent) as shown in Figure 1. The objective of the process is to remove radioactive cesium from the aqueous waste so that the decontaminated waste can be disposed of in the Saltstone facility, and the cesium-containing ion exchange material can be disposed of in the vitrified waste form from DWPF. The feed is first filtered through a module in one tank, then transferred to a module in the second tank containing the ion exchange column where cesium removal occurs. The waste that is fed to the ion exchange module and the decontaminated waste are transferred in pipes that are above the tank top. The decontaminated waste passes through a gamma monitor above the tank and immediately adjacent to the ion exchange module. The column is loaded with IONSIV<sup>®</sup> IE-911 (commercially available engineered form of CST), a granular material consisting of CST powder bound with an inorganic inert binder. The CST selectively and irreversibly removes cesium, including radioactive Cs-137, from the aqueous salt solution. To meet the particle size criteria for the DWPF, the cesium-loaded spent sorbent must be ground to a fine powder; this size reduction is accomplished in a grinder module in a second waste tank riser. The spent IE-911 is sluiced from the ion exchange module to the grinder module through an above-tank pipe. The ground IE-911 is dumped into the waste tank, where it is mixed with sludge, and eventually sent to DWPF. The specification for acceptability of the ground IE-911 is the same as for the frit;  $\leq 2$  wt% at > 80 mesh;  $\leq 10$  wt% at > 200 mesh.

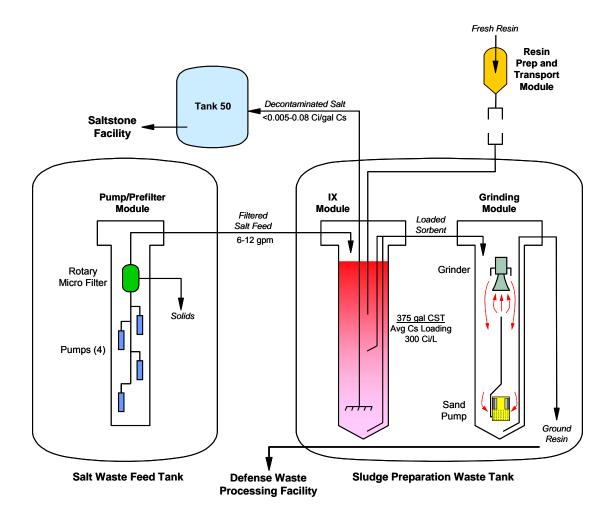


Figure 1. Schematic of the SCIX System

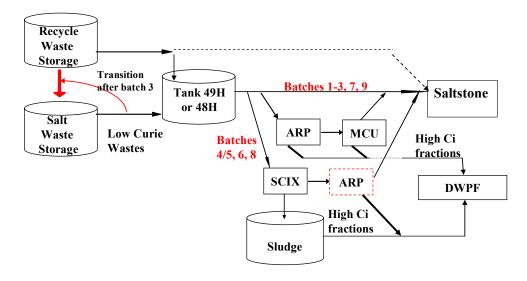
The design of the SCIX system has recently been revised to reduce the weight (McCabe and Phillips, 2004). Tank top loads are restricted, and construction of structures to distribute the weight off the tank top is expensive and adds to the duration of the installation schedule. The newly designed ion exchange bed is 27 inches in diameter and 13 feet tall, with a 6-inch diameter cooling pipe running vertically through the center, (i.e., contains 375 gallons of IE-911 material), and meets the weight restriction with a small margin. The expected operating flow rate ranges from 6 to 15 gpm of salt solution. Although in theory two columns could be operated in series (i.e., in a carousel fashion) to increase the Decontamination Factor and minimize IE-911 usage, this study assumes single column operation.

### 1.3 SCIX Waste Treatment Selection Methodology

To identify a conceptualized implementation plan for SCIX, it is necessary to examine current plans at SRS for waste sampling, dissolution, transfer, storage, treatment, disposal, budgets, process capacities, schedules, achievable decontamination targets, material compatibilities, and regulations. Technical matters to be addressed include aqueous waste and sludge batch

compositions. Although many of these parameters are not finalized in the SRS baseline, it is possible to perform a comparison to the baseline assumptions using the same inputs. The impact of some parameters must be postponed at this early stage of evaluation, such as the availability of transfer lines, sample analysis results, budgets, retrieval pumps, regulatory approval, etc. Although some of these support functions are not projected to be available because they are not within the needs for the current baseline, it is assumed for this evaluation that redirection of resources could make them available. This evaluation focuses on several key parameters: (a) availability of aqueous waste; (b) composition of the aqueous waste; (c) achievability of the target decontamination factor; (d) aqueous waste treatment rate; (e) IE-911 usage rate; (f) Saltstone impact; and (g) DWPF canister impact.

The proposed interim planning strategy baseline for SRS tank waste includes consideration of disposition of some low curie aqueous wastes in the Saltstone facility (Mahoney and d'Entremont, 2004). This flowsheet should be considered preliminary, and is not yet approved. The tank waste inventory and accounting is managed using the software SpaceMan Plus TM. The proposed changes to the portion of the flowsheet that would be affected by SCIX are shown in Figure 2. It is unlikely that SCIX could be constructed and installed earlier than December, 2006, so treatment of earlier batches was not considered. In this scenario, the flowsheet is unchanged through Saltstone Batch 3, and the SCIX begins operations on Saltstone Batches 4 and 5 together (designated as Batch 4/5). After Saltstone Batch 4/5 begins processing in SCIX. the Recycle waste from DWPF could be used for dissolution of saltcake, although the logistics of performing this were not evaluated here and are assumed viable. In the baseline, Batches 4 and 5 are comprised of 2.3 million gallons of liquid dispositioned in Saltstone with [Na<sup>+</sup>] at 3.3 M. Saltstone Batches 4 and 5 are identical in composition before Recycle is added, so the SpaceMan Plus<sup>™</sup> output stream is computed while the material is still in interim storage in Tank 49H. Batches 6 and 8 are currently being considered for treatment in the Actinide Removal Process (ARP) and Modular Caustic Side Solvent Extraction Unit (MCU) process. These streams were selected for this evaluation in order to perform a direct comparison of costs and benefits. The ARP and MCU process effluents to Saltstone are 1.44 million and 1.40 million gallons for Batches 6 and 8, respectively, with [Na<sup>+</sup>] at 4.8 M. The SpaceMan Plus<sup>™</sup> output stream used for this evaluation is the feed into the ARP process, which is at ~6.5 M [Na<sup>+</sup>]. It is not known if any of these streams will require a monosodium titanate (MST) addition to remove alpha contaminants, and it is possible that filtration alone will be sufficient. If MST addition is needed, the scenario evaluated here will need adjustment to allow time for the facility to initiate operations. Further, the impacts to the projected operating windows for DWPF performed in this study does not include titanium added from an MST process, and revisions to this would also be needed if MST is added.



\*streams that are not impacted are omitted for clarity

Figure 2. Potential SCIX Implementation Flowsheet

Five key parameters for this evaluation are the quantity and composition of the aqueous waste, the required Decontamination Factor, and the sludge quantity and composition. These variables directly impact the IE-911 usage rate and DWPF canister count. The aqueous waste composition was obtained from a run of the SpaceMan Plus M software model for SRS using the assumed planning baseline flowsheet (Elder, et al., 2004) with the version that was most up to date at the time. There are numerous assumptions contained within this computer model, and none were changed for this evaluation versus the baseline. The software tracks the composition and volume of the waste streams as part of its operation. After examining the planning baseline schedule, three waste streams were selected from the SpaceMan Plus M run for input to the ion exchange column modeling, designated as Saltstone Batches 4/5, 6, and 8. The salt solution in all of these batches originates primarily in Tanks 25H and 41H.

### 1.4 Aqueous Waste Compositions

The SpaceMan Plus<sup>TM</sup> model is used to simulate the HLW inventory by accounting for processing of salt and sludge using various scenarios within existing constraints, such as tank space (Elder, et al., 2004). SpaceMan Plus<sup>TM</sup> simulates all of the facilities in the Liquid Waste

and Waste Solidification System, including future facilities such as MCU and ARP (but currently not SCIX). SpaceMan Plus ™ uses the existing waste tank inventory and facility processing rates; variables can be entered to develop a processing scenario. It creates an initial snapshot of the entire HLW system, showing volumes, compositions, and operation of the various processes, then sequentially calculates snapshots of the system at weekly intervals, using the desired scenario. The program performs a material balance at each interval and continues for the entire time period of interest. Calculations are done in 1 week increments, so interface issues of less than 1 week duration are not detected. The program will not simulate operations that violate limits (e.g. transferring waste into a full tank or operating a process above its maximum capacity). So that the program will run quickly, it uses simplified versions of the flowsheet for each unit process. The output from the run includes composition and volume of each waste tank.

Information for this SCIX strategy evaluation was obtained by selecting the tank compositions at appropriately selected time intervals from a SpaceMan Plus TM run of the baseline planning flowsheet (Mahoney and d'Entremont, 2004). The output compositions from the SpaceMan Plus <sup>™</sup> run include soluble and insoluble species. The insoluble solids were assumed removed by the filter, so were not utilized. The soluble species were used in the CST absorption isotherm modeling with ZAM (Zheng, et al, 1996 and 1996a). This model generates the cesium equilibrium absorption curves over a range of cesium concentrations for a specified chemical composition and temperature. The species listed as soluble included over eighty chemical and radioactive species. Since ZAM only uses seventeen species in the input file, the SpaceMan Plus<sup>™</sup> output was reduced to those pertinent to ZAM. Minor adjustment of the ionic balance using nitrate ion was then performed to obtain a charge-neutral composition input file (a ZAM input requirement). Next, Batch 4/5 was diluted from 8.0 M to 7.0 M [Na<sup>+</sup>] to meet the Saltstone Waste Acceptance Criteria (WAC), to improve the cesium absorption, and to reduce the viscosity of the fluid. Since the feed pumps for the SCIX must push the liquid through the filter, through the ion exchange bed, and out to the receipt tank, high viscosity will negatively impact throughput performance. The diluted, charge-balanced compositions of the three batches are shown in Table 1, along with the nominal amount of nitrate that was changed to achieve a charge balance when the composition was reduced to the ZAM components. Note that three ZAM component inputs were "0" and are not shown in Table 1; H<sup>+</sup>, Rb<sup>+</sup>, and Sr(OH)<sup>+</sup> (The [H<sup>+</sup>] is insignificant at very high pH, the [Rb<sup>+</sup>] is unknown, and ZAM calculates the Sr(OH)<sup>+</sup> concentration from the [OH] and Sr<sup>+2</sup> concentrations). Also note that the Cs-137 to nonradioactive cesium ratio is not quite constant because of differences in the ages of the waste. The ion exchange sorbent will remove both radioactive and non-radioactive cesium indiscriminately, so both must be tracked in the modeling. Also, strontium is a significant competitor for cesium absorption on the ion exchange sorbent. Normally, the quantity of total strontium is insignificant, but the SpaceMan Plus<sup>TM</sup> output shows a relatively high value for Batch 8, where it exceeds the cesium concentration. While it is expected that this would actually exceed the strontium solubility limit and therefore be removed by filtration, the listed value was used in the ZAM modeling to ensure a conservative outcome.

**Table 1. Batch Compositions used for Column Modeling** 

| Ion<br>Category           | Species                       | Batch 4/5<br>Diluted | Batch 6   | Batch 8   |
|---------------------------|-------------------------------|----------------------|-----------|-----------|
| Category                  |                               | [M]                  | [M]       | [M]       |
| Cations*                  | Na <sup>+</sup>               | 7.00                 | 6.44      | 6.54      |
|                           | Total Cs <sup>+</sup>         | 2.455E-05            | 7.769E-05 | 3.962E-05 |
|                           | Cs-137<br>(Ci/gal)            | 0.37                 | 1.00      | 0.64      |
|                           | K <sup>+</sup>                | 0.0119               | 0.0302    | 0.0165    |
|                           | Sr <sup>2+</sup>              | 9.407E-06            | 1.695E-06 | 4.913E-05 |
|                           | Ca <sup>2+</sup>              | 1.257E-04            | 7.891E-05 | 2.588E-05 |
| Anions                    | OH <sup>-</sup> (free)        | 0.757                | 1.744     | 3.627     |
|                           | NO <sub>3</sub>               | 5.009                | 3.604     | 1.558     |
|                           | NO <sub>2</sub> -             | 0.179                | 0.369     | 1.009     |
|                           | Cl                            | 0.002                | 0.004     | 0.003     |
|                           | F <sup>-</sup>                | 0.017                | 0.014     | 0.003     |
|                           | Al(OH) <sub>4</sub>           | 0.143                | 0.167     | 0.039     |
|                           | CO <sub>3</sub> <sup>2-</sup> | 0.310                | 0.192     | 0.130     |
|                           | SO <sub>4</sub> <sup>2-</sup> | 0.113                | 0.069     | 0.019     |
|                           | PO <sub>4</sub> <sup>3-</sup> | 0.020                | 0.016     | 0.007     |
| Isotope<br>Fraction       | Cs-137                        | 0.337                | 0.284     | 0.357     |
| Nitrate<br>adjustment +/- |                               | 0.00406              | -0.05565  | -0.01987  |

### 1.5 SCIX Column Modeling

The tank waste compositions were input to the ZAM computer model (Zheng, 1996) to generate cesium absorption isotherms. The isotherms were then used for input to the VERSE model to generate breakthrough profiles. These techniques have been used elsewhere and shown to give reasonable performance predictions (Hamm, et al; 1999, 2002, 2003). Output from the VERSE code was used to calculate the number of columns of IE-911 needed to decontaminate the aqueous waste. Two exit criteria were used, 0.08 Ci/gal and 0.005 Ci/gal, both using a "bucket average" value for the target, i.e., the calculated average effluent concentration if the liquid was composited. The 0.08 Ci/gal target was selected for comparison to prior estimates, and the 0.005

Ci/gal target is marginally below the Nuclear Regulatory Commission Class A waste disposal limit.

### 1.6 Sludge Batch Selection Methodology

The quantity of IE-911 that is projected to be loaded with cesium was then used in modeling of the DWPF glass chemistry. To do this, it was first necessary to determine a reasonable projection of when the spent IE-911 would be available, which tank the IE-911 and sludge would be in, what sludge is being processed in DWPF and its composition, and the timing of transfers. The current concept for SCIX assumes that the column and grinder would be located in Tank 51H. As stated above, the SCIX is not expected to be implemented before December, 2006. In 2007, it is anticipated that a heel of washed Sludge Batch 4 (SB4) will be present in Tank 51H, as the majority of SB4 is being fed to DWPF from Tank 40H. It is expected that in late 2007, the heel in Tank 51H will be transferred into Tank 40H. Therefore, for this evaluation it was assumed that the entirety of the IE-911 from processing the three batches described above would be mixed with a full tank of SB4. Depending on the flow rate through the filter and ion exchange unit and actual timing of sludge processing, the full amount of IE-911 may not be available by the time this heel transfer occurs. The remainder of the IE-911 would then be mixed with Sludge Batch 5. Schedule slippage in any of these implementation plans would impact the mixing scenario, and it is not possible to predict exactly what will happen. However, despite several potential variables, it was concluded that assessments of projected operating windows via the model-based process control system should be done with SB4; because this is the most likely scenario and the chemical composition of this batch is known with higher confidence than Sludge Batch 5. The glass model-based assessments are based on a tentative (or preliminary projected) composition of SB4, sludge retrieval strategy refinement and sample analysis results will improve the confidence of the projected composition. Further glass chemistry model based assessments of the impacts to DWPF will be needed when the schedules, composition, and sludge volumes are better defined.

#### 1.7 Conversion of IE-911 to Waste Oxide Mass

The ZAM modeling is based on equilibrium chemistry with the powdered CST, not the granular engineered form with its inert binder, which is the form that is planned for SCIX. It appears that the ZAM model uses the weight of the hydrogen form of the CST, based on comparison of K<sub>d</sub> values using both hydrogen and sodium input forms. To calculate the amount of waste oxides, results from ZAM were first converted for use in VERSE using a "dilution factor" that accounts for the effect of the binder, assumed at 32 wt% (see Hamm et al., 2002). The VERSE model calculates the quantity of waste that can be treated per column, which is then converted to the number of columns (and quantity of IE-911 spent) used for a given waste volume. For the glass chemistry model-based assessments associated with the DWPF projected operating windows, the input files must be in terms of "waste oxide", i.e., the form of elemental oxide present in the final glass waste form. Since ZAM uses the hydrogen form of IE-911, the elemental composition of the spent form must be adjusted to account for the added sodium ions. The quantity of loaded IE-911 generated from VERSE modeling was then converted to the sodium form and calculated as a mass of elemental oxides. The elemental composition used for the spent IE-911 was based on analysis results of IONSIV® IE-911 in the caustic-washed (leached) form (Nyman, et al., 2001). This leaching both converts the hydrogen form of the material to the sodium form and removes excess constituents from manufacturing. The calculation of waste oxide mass from

spent IONSIV<sup>®</sup> IE-911 includes the tacit assumption that the chemical speciation converts from IE-911 to those species normally in borosilicate glass (e.g. sodium present as Na<sub>2</sub>O).

### 1.8 Model-Based Assessments of Projected Glass Operating Windows

The impacts of SCIX on the DWPF were assessed relative to a baseline sludge-only flowsheet and include processing issues associated primarily with the DWPF Chemical Process Cell (CPC), projected glass operating windows (which are based on model predictions and are represented in terms of waste loading (WL) intervals), and canister production totals. Glass chemistry modeling was performed using the constraints of the PCCS (Brown, Postles, and Edwards, 2002), and therefore mimics the control system used by DWPF in glass production. The model evaluates the impact of elemental compositions on the projected operating window (i.e., defines the upper and lower waste loadings that produce an acceptable glass based on model predictions). Frit 320 was used for this evaluation since it was used previously for modeling SB4 impacts, and it has been found to have broad applicability as well as the potential to improve waste throughput at DWPF. This frit may not be optimal for either SB4-only processing or SB4-IE-911 (coupled) processing. Whether the impact of the results will translate to another frit formulation is not known. The waste loadings presented provide a relative measure of the impact of SCIX and associated volume on the operational flexibility and potential maximum waste loadings that could be attained in DWPF using a fixed frit composition. Based on the projected operating windows, assessments are made with respect to potential impacts to canister production totals. No experimental work (including assessments of melt rate) was performed as part of this assessment, so parameters that have not been previously studied could not be addressed.

The impact of titanium on DWPF glass production volume has been an area of considerable concern because titania has a marginal solubility in borosilicate glass. The primary sources of titania in the system are the sludge and MST from the ARP. However, since the impact of the IE-911 material was the focus of this study and the exact volumes and timing of MST from ARP to be transferred to DWPF during SB4 are not known, the effect of MST from the ARP was not included in the evaluation. Once the volumes and timing of the SCIX material and the ARP material are determined for the particular sludge batch, further assessments of the titania limit should be performed. For this evaluation, the current PCCS limit of 1 wt% titania was replaced with a 2 wt% limit, if no other product quality limits were exceeded. Although glass quality experimental evidence exists for raising the limit (Lorier 2003), other factors, such as impact on melt rate, have not been determined.

Composition of SB4 was derived from a report using an assumed sludge mixing plan (Lilliston, 2004). The volume and composition of SB4 are subject to change, based on new strategies, chemical analyses, tank volume estimates, and other factors. This evaluation represents a snapshot of projections in composition, volumes, and schedules, and a new evaluation will be needed when more information is obtained. Mixing of ground IE-911 with SB4 using the current in-tank slurry pumps is assumed to be a viable method for homogenizing the mixture.

Impact on the DWPF CPC was evaluated by judging the estimated parameters against known system constraints, no experimental work was performed. Glass waste loading limits were obtained from the PCCS models, and previous studies have examined some sludge-IE-911

characteristics (Hansen et al., 2001; Baich, 2000). This information allowed estimates of changes in sludge slurry volume and characteristics, and the results were used to judge the impact on the CPC. Parameters of concern that contribute to the operational flexibility of the CPC include rheology, water evaporation rate, acid reactivity, and representative sampling. While some experimental work has been performed on similar waste streams (Edwards, et al., 1999), further work would be needed to confirm the CPC evaluation conclusions.

The impact of SCIX on the DWPF melt rate cannot be predicted at this time. No models or correlations exist that can be used to establish a basis for melter throughput. Also, there is no information available on the impact of  $Nb_2O_5$  (a material unique to CST) on the glass liquidus temperature. Experimental work would be needed to develop the necessary information regarding impacts to melt rate and/or liquidus temperature modeling prior to implementation.

# 2.0 Column Performance Projection

Computer modeling was performed to project the performance of the proposed IE-911 small column design. The SCIX design has evolved as requirements have become defined, and the design used here has been used in a previous study (for further details see Aleman and Hamm, 2003, Rev. 1). Column performance modeling was completed for three feed solutions at two different flow rates. Post-modeling calculations for cesium breakthrough performance and cesium inventories were also performed and are provided in this chapter. For these post-modeling calculations, results are provided for conditions with exit breakthrough criteria of 0.005 and 0.08 Ci/gal. All assumptions and most parameters identified in the previous report (Aleman and Hamm, 2003, Rev. 1) are valid here (such as: the density of the material; porosity; cesium diffusivity; binder effects; etc.) unless otherwise noted.

### 2.1 Column Design and Performance Scenarios Analyzed

The most recent design for the SCIX was used in this study, where the IE-911 bed is 27½ inches in diameter and 13 feet long, containing 375 gallons of sorbent. This column design has water cooling through the center of the column using a 6 inch outer diameter pipe. Table 2 is a summary of the column design (i.e., design #6 from Aleman and Hamm, 2003, revision 1) used in this report. "Design 6" provides the actual dimensions of the proposed design, while the "design 6 (equiv vol)" provides the equivalent volume dimensions actually used in the VERSE simulation runs (Whitley, Wang, 1998). This mathematically accounts for the geometry of the center cooling pipe, which effectively reduces the column diameter for the VERSE input files.

For this column design, six column performance scenarios were evaluated; three feed compositions at two flow rates (i.e., 6 and 15 gpm). Table 3 provides a list of the six column performance scenarios used. The VERSE simulations were allowed to run beyond the desired cesium exit criterion in order to post-calculate column performance and inventory for two different exit criteria (i.e., bucket averages of 0.005 and 0.08 Ci of Cs-137/gal).

| 1 able | 2. IE-91 | 1 Ion Excha | nge Column | Desig | n Stuu | ieu |
|--------|----------|-------------|------------|-------|--------|-----|
| <br>   | _        |             |            |       | -      |     |

| Column        | Column | Outer    | Outer Core |        | Inner Core | Column | Column   |
|---------------|--------|----------|------------|--------|------------|--------|----------|
| Design        | Length | Diameter | Wall       | ID     | OD         | L/D    | Volume   |
|               | (ft)   | (in)     | (in)       | (in)   | (in)       |        | (gal/L)  |
| 6             | 13.0   | 27.250   | 0.0        | 27.250 | 6.0        | 5.7    | 375/1419 |
| 6 (equiv vol) | 13.0   | 26.581   | 0.0        | 26.581 | 0.0        | 5.9    | 375/1419 |

**Table 3. Column Performance Scenarios Analyzed** 

| Scenario | Tank              | Feed       | Feed     |
|----------|-------------------|------------|----------|
| No.      | Feed              | Flow (gpm) | Temp (C) |
| 1        | Batch 4/5 Diluted | 15         | 30       |
| 2        | Batch 4/5 Diluted | 6          | 30       |
| 3        | Batch 6           | 15         | 30       |
| 4        | Batch 6           | 6          | 30       |
| 5        | Batch 8           | 15         | 30       |
| 6        | Batch 8           | 6          | 30       |

### 2.2 Waste Compositions

Table 1 lists the three salt waste compositions utilized in this work. The calculated fraction of Cs-137 to total cesium is also shown, which was calculated using the specific activity of Cs-137 of 87 Ci/g (ORNL, 1995). The Sr<sup>2+</sup> species were entered into ZAM directly, where ZAM then computes its equilibrium value with Sr(OH)<sup>+</sup>, which competes with Cs<sup>+</sup> for some of the available CST sites (see Hamm et al., 2002).

### 2.3 Cesium Absorption Isotherms

A three step process generated the cesium sorption data in a form suitable for column modeling. First, the ZAM model is used to calculate equilibrium data for cesium absorbed onto powdered CST (IONSIV® IE-910) for each of the specific waste compositions listed in Table 1. Second, the IE-910 data were fitted to an algebraic equation for each case study. Third, a dilution factor applied to the IE-910 fitted equation provided an offset for estimating IONSIV® IE-911 performance (i.e., the granular form), and represents "dilution" of CST by the binder. Column modeling with the VERSE-LC code used the IE-911 isotherms.

Cesium loading curves (i.e., isotherms at 30 °C) were generated for IE-910 and IE-911. The ZAM model calculated the loading data for IE-910 using the solution compositions given in Table 1. Figures were generated showing the ZAM data and algebraic fit of the data. These included the isotherm fitted to the ZAM data (IE-910) and an isotherm for IE-911. The IE-911 isotherm is offset because of the applied "dilution" factor. The 68% dilution factor applied to the ZAM results represents a 32% lower capacity of IE-911 compared to ZAM predictions.

Experimental data indicate that this is a conservative estimate of the magnitude of this dilution factor (Hamm et al., 2002).

Figures 3 through 5 represent the cesium isotherms for Batch 4/5 Diluted, Batch 6, and Batch 8 waste solutions, respectively. The nominal cesium feed concentration for each waste stream is also plotted along with the isotherms in each figure. In Figure 6 a comparison of all three isotherms is shown. The isotherm corresponding to the Batch 4/5 Diluted waste stream is the most demanding of the three, despite the high Sr in Batch 8. The reason for this is the higher sodium concentration and lower hydroxide concentration in Batch 4/5. As can be seen in Figure 6 and from Table 4, the isotherms follow the trend associated with sodium concentration level. These isotherms are considered to be at nominal values (i.e., most parameter settings were set to their best estimate values except the dilution factor which was set to a statistically conservative value of 68%).

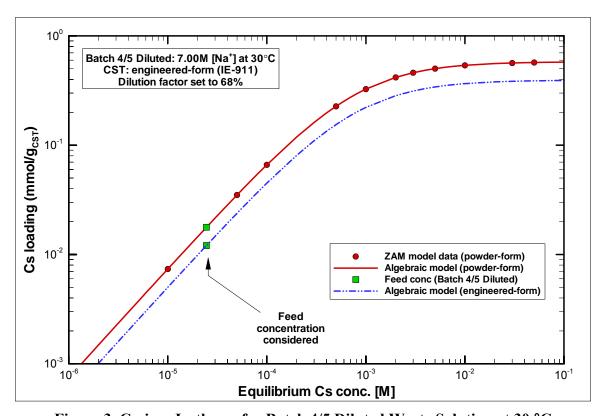


Figure 3. Cesium Isotherm for Batch 4/5 Diluted Waste Solution at 30 °C

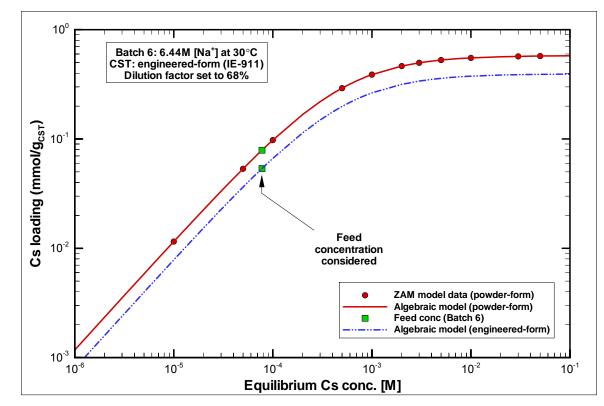


Figure 4. Cesium Isotherm for Batch 6 Waste Solution at 30 °C.

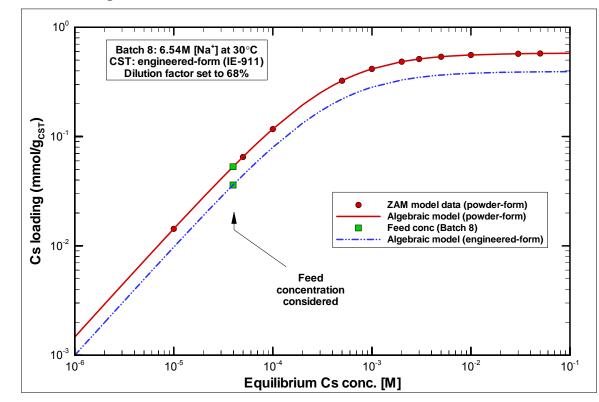


Figure 5. Cesium Isotherm for Batch 8 Waste Solution at 30 °C

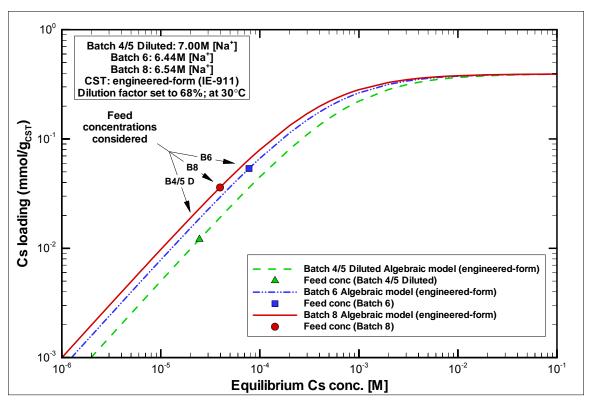


Figure 6. Cesium Isotherm Comparison of the Three Waste Solutions at 30 °C

### 2.4 Column Performance Modeling

The VERSE-LC computer code performed the cesium ion exchange modeling for columns packed with IONSIV® IE-911 (Whitley and Wang, 1998). This transport model includes axial dispersion, film diffusion, and pore diffusion within the IE-911 particles. Given column, transport, and operating parameters, the VERSE-LC code provides the cesium concentration in the column effluent as a function of the volume of waste processed; referred to as a "breakthrough curve".

Two formats were used for plotting breakthrough curves, instantaneous exit concentration and "bucket average". The first format plots the instantaneous exit concentration of cesium leaving the column as a function of the volume of salt solution processed. The second format plots the volume-averaged cesium concentration of the processed solution (i.e., "bucket average"). The first format fits a process controlled by a limiting value of the cesium concentration at the column exit. For example, if the product must contain less than 0.08 Ci of Cs-137 per gallon of processed waste, this control method stops processing when the instantaneous exit concentration equals the 0.08 Ci/gal limit. In this case, the entire batch of processed waste averages much less than 0.08 Ci/gal since only the final drop equaled 0.08 Ci/gal. An alternative process control strategy monitors the volume (mixture) average cesium concentration of the batch of waste passed through the column and ensures the batch average (or "bucket" average) does not exceed 0.08 Ci/gal. This alternative allows processing more waste through a column and generates less loaded sorbent to be disposed of within the melter. This latter process strategy was used for subsequent calculations regarding the quantity of IE-911 needed and volume of waste treated.

Tables 4 and 5 summarize the volume of waste processed for three batches of feed solution at a cesium breakthrough of 0.005 and 0.08 Ci/gal, respectively. The instantaneous and bucket average cesium breakthrough curves at 6 and 15 gpm are shown in Figures 7 and 8, respectively. Figure 7 shows the cesium breakthrough curves for the Batch 4/5 Diluted, Batch 6, and Batch 8 waste compositions at a flow rate of 6 gpm. The order of breakthrough (first to last), from Batch 4/5 Diluted to Batch 8, is consistent with the cesium isotherm comparison shown in Figure 6. The Batch 4/5 Diluted cesium isotherm has the lowest cesium loading for a given aqueous cesium concentration and the Batch 8 cesium isotherm has the highest cesium loading. The waste volume processed can be determined for any decontamination factor desired. For example, assuming a product limit of 0.08 Ci/gal, requires a Decontamination Factor of 4.6, 12.5, and 8.0 for Batch 4/5 Diluted, Batch 6, and Batch 8 waste solutions, respectively. From the curves in Figure 7, a 375-gal column operating at a flow rate of 6 gpm with Batch 4/5 Diluted, Batch 6, and Batch 8 waste compositions will process 228, 259, and 367 kilo-gallons, respectively, at a bucket average cesium breakthrough of 0.08 Ci/gal. From the curves in Figure 8, the same column operating at a flow rate of 15 gpm with Batch 4/5 Diluted, Batch 6, and Batch 8 waste compositions will process 209, 219, and 321 kilo-gallons, respectively, at a bucket average cesium breakthrough of 0.08 Ci/gal.

Table 4. Volume of Waste Processed for the Three Feed Solutions at a Cesium Breakthrough of 0.005 Ci/gal

| Scenario | Figure | Tank              | Feed  | Feed | Volume<br>Processed | Volume<br>Processed |
|----------|--------|-------------------|-------|------|---------------------|---------------------|
| No.      |        | Feed              | Flow  | Temp | Exit                | Bucket              |
|          |        |                   | (gpm) | (C)  | (kgal)              | (kgal)              |
| 1        | 8      | Batch 4/5 Diluted | 15    | 30   | 62                  | 90                  |
| 2        | 7      | Batch 4/5 Diluted | 6     | 30   | 97                  | 129                 |
| 3        | 8      | Batch 6           | 15    | 30   | 86                  | 119                 |
| 4        | 7      | Batch 6           | 6     | 30   | 138                 | 177                 |
| 5        | 8      | Batch 8           | 15    | 30   | 113                 | 160                 |
| 6        | 7      | Batch 8           | 6     | 30   | 179                 | 234                 |

Table 5. Volume of Waste Processed for the Three Feed Solutions at a Cesium Breakthrough of 0.08 Ci/gal

| Scenario<br>No. | Figure | Tank<br>Feed      | Feed<br>Flow<br>(gpm) | Feed<br>Temp<br>(C) | Volume<br>Processed<br>Exit<br>(kgal) | Volume<br>Processed<br>Bucket<br>(kgal) |
|-----------------|--------|-------------------|-----------------------|---------------------|---------------------------------------|---|
| 1               | 8      | Batch 4/5 Diluted | 15                    | 30                  | 122                                   | 209                                     |
| 2               | 7      | Batch 4/5 Diluted | 6                     | 30                  | 146                                   | 228                                     |
| 3               | 8      | Batch 6           | 15                    | 30                  | 143                                   | 219                                     |
| 4               | 7      | Batch 6           | 6                     | 30                  | 188                                   | 259                                     |
| 5               | 8      | Batch 8           | 15                    | 30                  | 201                                   | 321                                     |
| 6               | 7      | Batch 8           | 6                     | 30                  | 255                                   | 367                                     |

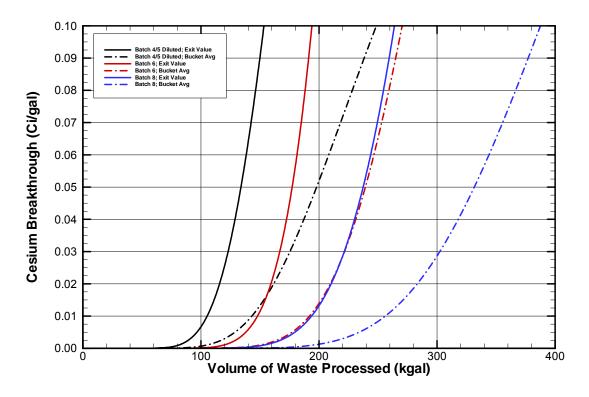


Figure 7. Cesium Breakthrough Curves for the Salt Solutions at 30 °C and 6 gpm.

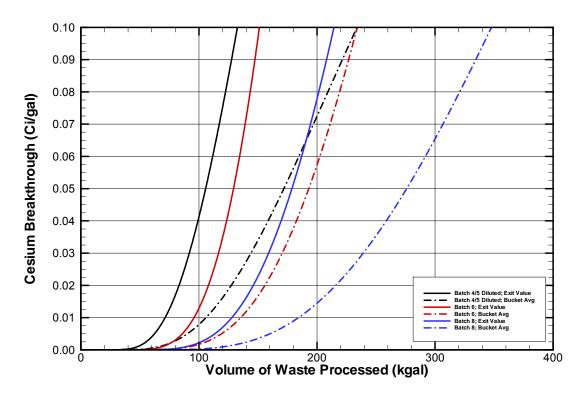


Figure 8. Cesium Breakthrough Curves for the Salt Solutions at 30 °C and 15 gpm

### 2.5 Cesium Column Inventory Analysis for IE-911

The average Cs-137 column loading and the axial Cs-137 loading profile was computed for IE-911 at the point where the bucket average cesium breakthrough met the exit criterion of 0.005 and 0.08 Ci/gal. Since there is some indication that absorption performance of CST in its engineered form is comparable to computer projections of un-bound, powdered CST (Wilmarth, et al., 2001) both column inventory nominal estimates (i.e., dilution factor set to 68%) and conservative estimates (i.e., dilution factor set to 100%) were computed. The "68%" and "100%" refer to the concentration of CST in IE-911, i.e., 32% binder and 0% binder, respectively. For column performance with respect to estimating an upper limit on spent IE-911, the results associated with a dilution factor of 68% is appropriate. For column performance with respect to estimating an upper limit of cesium inventory, the results associated with a dilution factor of 100% is appropriate. The average Cs-137 loadings for the three feed solutions are summarized in Tables 6 and 7 for the bucket average exit criterion value of 0.005 and 0.08 Ci/gal, respectively. The nominal and conservative estimates of the axial Cs-137 loading profile for IE-911 are shown in Figures 9 to 14 for the breakthrough curves shown above. The axial cesium loading was computed from the corresponding axial aqueous cesium concentration using the appropriate algebraic isotherm. The axial Cs-137 loading was computed from the axial cesium loading using an IE-911 bulk density of 1.0 g/mL, specific activity of Cs-137 (87 Ci/g) and assuming the appropriate Cs-137 isotopic fraction value as listed in Table 1. One sample VERSE input file for each waste stream considered is provided in Appendix A. These input files correspond to column design 6 at 30° C and 15 gpm.

Table 6. Column Average Cs-137 Loading for the Three Tank Feed Solutions at a Cesium Breakthrough of 0.005 Ci/gal (bucket average criterion employed).

| Scenario<br>No. | Figure    | Tank<br>Feed      | Feed<br>Flow<br>(gpm) | Feed Temp (C) | Cs-137<br>Loading<br>IE-911<br>(Ci/L) | Cs-137<br>Loading<br>IE-910<br>(Ci/L) |
|-----------------|-----------|-------------------|-----------------------|---------------|---------------------------------------|---------------------------------------|
| 1               | 9         | Batch 4/5 Diluted | 15                    | 30            | 23                                    | 34                                    |
| 2               | Not shown | Batch 4/5 Diluted | 6                     | 30            | 33                                    | 49                                    |
| 3               | 11        | Batch 6           | 15                    | 30            | 83                                    | 122                                   |
| 4               | Not shown | Batch 6           | 6                     | 30            | 124                                   | 182                                   |
| 5               | 13        | Batch 8           | 15                    | 30            | 72                                    | 105                                   |
| 6               | Not shown | Batch 8           | 6                     | 30            | 105                                   | 154                                   |

Table 7. Column Average Cs-137 Loading for the Three Tank Feed Solutions at a Cesium Breakthrough of 0.08 Ci/gal (bucket average criterion employed).

| Scenario | Figure    | Tank              | Feed  | Feed | Cs-137<br>Loading | Cs-137<br>Loading |
|----------|-----------|-------------------|-------|------|-------------------|-------------------|
| No.      |           | Feed              | Flow  | Temp | IE-911            | IE-910            |
|          |           |                   | (gpm) | (C)  | (Ci/L)            | (Ci/L)            |
| 1        | 10        | Batch 4/5 Diluted | 15    | 30   | 43                | 64                |
| 2        | Not shown | Batch 4/5 Diluted | 6     | 30   | 47                | 69                |
| 3        | 12        | Batch 6           | 15    | 30   | 141               | 208               |
| 4        | Not shown | Batch 6           | 6     | 30   | 167               | 246               |
| 5        | 14        | Batch 8           | 15    | 30   | 126               | 186               |
| 6        | Not shown | Batch 8           | 6     | 30   | 144               | 212               |

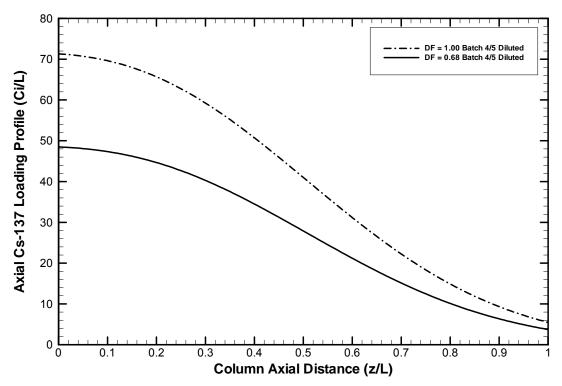


Figure 9. IE-911 Axial Cs-137 Loading Profile for Batch 4/5 Diluted (Bucket Average Criterion of 0.005 Ci/gal, 30°C, and 15 gpm)

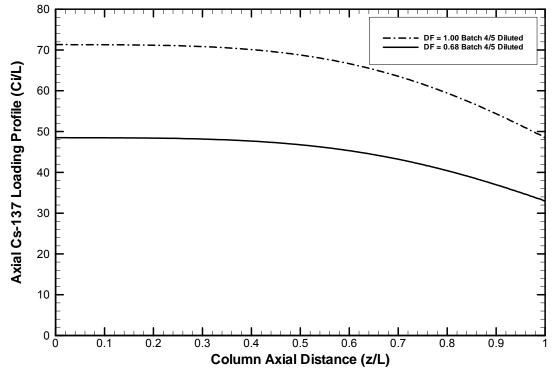


Figure 10. IE-911 Axial Cs-137 Loading Profile for Batch 4/5 Diluted (Bucket Average Criterion of 0.08 Ci/gal, 30°C, and 15 gpm))

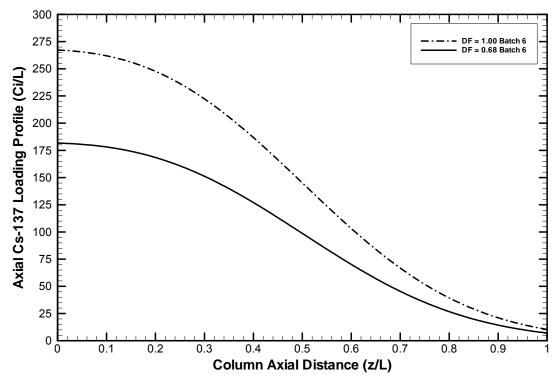


Figure 11. IE-911 Axial Cs-137 Loading Profile for Batch 6 (Bucket Average Criterion of 0.005 Ci/gal, 30°C, and 15 gpm)

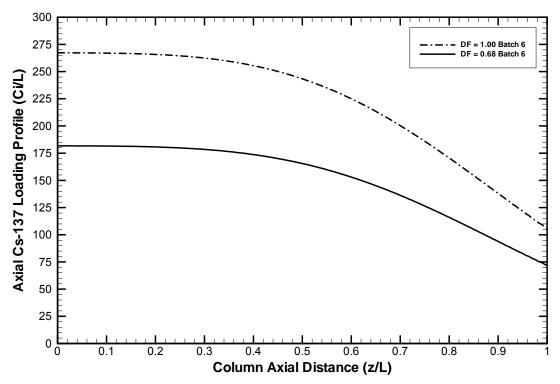


Figure 12. IE-911 Axial Cs-137 Loading Profile for Batch 6 (Bucket Average Criterion of 0.08 Ci/gal, 30 °C, and 15 gpm)

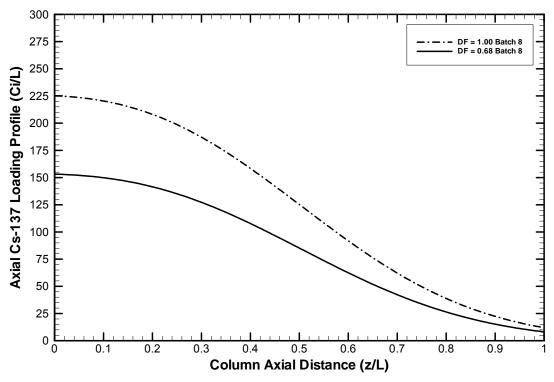


Figure 13. IE-911 Axial Cs-137 Loading Profile for Batch 8 (Bucket Average Criterion of 0.005 Ci/gal, 30°C, and 15 gpm)

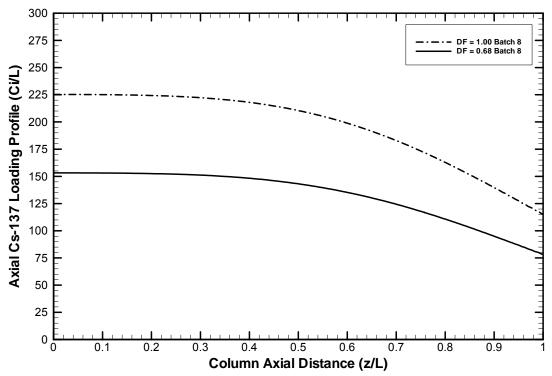


Figure 14. IE-911 Axial Cs-137 Loading Profile for Batch 8 (Bucket Average Criterion of 0.08 Ci/gal, 30°C, and 15 gpm)

# 3.0 IE-911 Usage and Processing Rates

The projected quantity of IE-911 generated in processing these batches of aqueous waste is summarized in Tables 8 (0.08 Ci/gal average effluent) and 9 (0.005 Ci/gal average effluent).

Table 8. Quantity of IE-911 Generated with 0.08 Ci/gal Effluent

| Parameter  | Batch 4/5<br>Diluted | Batch 6<br>Nominal | Batch 8<br>Nominal |
|--|----------------------|--------------------|--------------------|
| Batch Volume (kgal)                                | 1131                 | 959                | 1,121              |
| # Columns of IE-911 loaded at 15 gpm flow rate     | 6                    | 5                  | 4                  |
| # Columns of IE-911 loaded at 6 gpm flow rate      | 5                    | 4                  | 3                  |
| Cs-137 removed per column at 15 gpm flow rate (Ci) | 6.13E+4              | 2.01E+5            | 1.79E+5            |
| Cs-137 removed per column at 6 gpm flow rate (Ci)  | 6.70E+4              | 2.37E+5            | 2.05E+5            |
| Loaded IE-911 generated at 15 gpm flow rate (lbs)  | 18,780               | 15,650             | 12,520             |
| Loaded IE-911 generated at 6 gpm flow rate (lbs)   | 15,650               | 12,520             | 9390               |

Table 9. Quantity of IE-911 Generated with 0.005 Ci/gal Effluent

| Parameter  | Batch 4/5<br>Diluted | Batch 6<br>Nominal | Batch 8<br>Nominal |
|--|----------------------|--------------------|--------------------|
| Batch Volume (kgal)                                | 1131                 | 959                | 1,121              |
| # Columns of IE-911 loaded at 15 gpm flow rate     | 13                   | 8                  | 7                  |
| # Columns of IE-911 loaded at 6 gpm flow rate      | 9                    | 6                  | 5                  |
| Cs-137 removed per column at 15 gpm flow rate (Ci) | 3.32E+4              | 1.18E+5            | 1.02E+5            |
| Cs-137 removed per column at 6 gpm flow rate (Ci)  | 4.74E+4              | 1.75E+5            | 1.48E+5            |
| Loaded IE-911 generated at 6 gpm flow rate (lbs)   | 28,170               | 18,780             | 15,650             |

### 3.1 Cycle Time

In order to estimate schedule impacts, such as when the loaded IE-911 will be available and when the salt solution will be decontaminated, it is necessary to estimate the duration of a treatment cycle. The treatment cycle is defined as charging the fresh IE-911 into the column, loading (i.e., decontamination of salt solution until breakthrough), rinsing the spent IE-911, sluicing the first half of the bed into the grinder, grinding the first half of the bed, and sluicing the second half of the bed. It is assumed that grinding of the second half of the bed is not part of the cycle because, presumably, the empty column could be refilled while grinding occurs. The loading step is computed from the flow rate and volume of liquid that can be treated by a single column. All other steps are estimated to be completed within a total of 3 days. Total operating time availability is assumed to be 75% due to outages, non-routine maintenance, etc. Routine maintenance can be scheduled each time the feed batch is switched, which is expected to take about 2 weeks to fill the feed tank, so was not added as a separate item. The overall duration for each condition is shown in Table 10. Depending on the assumed flow rate and effluent activity target, the processing time for all three batches ranges from 28 to 91 weeks, including 4 weeks for refilling the feed tank twice.

**Table 10. Estimated Cycle Durations** 

| Parameter   | Batch 4/5 | Batch 6 | Batch 8 |
|---|-----------|---------|---------|
|   | Diluted   | Nominal | Nominal |
| Batch Volume (kgal)   | 1131      | 959     | 1,121   |
| Loading time at 15 gpm (days)                               |           |         |         |
|   | 4.2       | 5.5     | 7.4     |
| Loading time at 6 gpm (days)                                |           |         |         |
|   | 15.3      | 20.5    | 27.1    |
| Charge/discharge time (days)                                | 3         | 3       | 3       |
| Total cycle time at 15 gpm (days)                           | 9.6       | 11.4    | 13.9    |
| Total cycle time at 6 gpm (days)                            | 24.4      | 31.3    | 40.1    |
| Total Batch processing time at 15 gpm & 0.08 Ci/gal (weeks) | 8.2       | 8.1     | 7.9     |
| Total Batch processing time at 6 gpm & 0.08 Ci/gal (weeks)  | 17        | 18      | 17      |
| Total Batch process time at 15 gpm & 0.005 Ci/gal (weeks)   | 18        | 13      | 14      |
| Total Batch process time at 6 gpm & 0.005 Ci/gal (weeks)    | 31        | 27      | 29      |

#### 3.2 Waste Oxide to DWPF

In order to determine the impact on DWPF glass chemistry, the composition and quantity of IE-911 sent to DWPF must be determined. One column operating condition was selected in order to minimize the number of glass chemistry calculations needed. Although the bounding condition shown from the VERSE modeling is at 15 gpm and an effluent activity target of 0.005 Ci/gal, it is unlikely that this condition would be selected because of the high consumption rate of IE-911. If the high flow rate and low effluent target were needed, use of two columns in series would seem more efficient. Therefore, the condition chosen for glass modeling was with the lower effluent activity target (0.005 Ci/gal) and lower flow rate (6 gpm) as shown in the bottom row of Table 9. This would generate 20 columns (62,600 lbs) of IONSIV® IE-911, instead of the 28 columns using the bounding condition. Since this calculation originated with the ZAM/VERSE modeling, the quantity of material was converted to the sodium form before calculation to the waste oxide weight. The quantity of waste oxides sent to DWPF are expressed in terms of the form of the elemental oxides (Nyman, 2001) converted to the form expected in DWPF glass (Table 11). Displacing hydrogen with sodium in the CST matrix adds 5.7% to the total mass of material (Nyman, 2001), increasing the weight to 66,168 lbs. Note that some of the mass of material is lost as water and oxygen in the subsequent conversion from IE-911 to glass waste oxides, as can be seen in the non-normalized total of 89 wt% oxides. The calculated quantity of waste oxides generated from the column was then used in assessing the impact on glass chemistry in DWPF.

non-Oxide to **DWPF** normalized wt% wt% oxide Element atom wt oxide molec wt lbs 16.27 47.867 TiO<sub>2</sub> 79.847 27.140 17958 Τi Si 7.46 28.056 SiO<sub>2</sub> 60.036 15.963 10563 Zr 10.21 91.224  $ZrO_2$ 123.204 13.789 9124 Na 10.03 22.989 Na<sub>2</sub>O 61.968 13.518 8945 12464 13.17 92.906 Nb<sub>2</sub>O<sub>5</sub> 265.762 18.837 Nb 89.248 59053 sum

Table 11. Calculation of Waste Oxides to DWPF

### 4.0 DWPF Impact

For every sludge batch to be processed at DWPF or for any new stream that is to be immobilized at DWPF, an impact assessment is performed by a team consisting of facility personnel, the planning and integration group of the Closure Business Unit, and SRNL. The impact matrix includes such categories as segregation, criticality, and product quality with various concerns associated with each category. The team looks at the items identified and uses their judgment to determine whether engineering or experimental studies are required, the risk is acceptable, or prior process knowledge is sufficient to dismiss the risk. The objective of the impact assessment is to identify any risks/concerns before the sludge batch or new stream is processed. A similar

logic process was performed to evaluate the impact of the SCIX stream, but the focus was more limited to direct impacts on DWPF and to experimental work already performed. The following sections summarize this assessment.

### 4.1 Definition of Baseline Flowsheet and Alternative Sludge Stream Compositions

To assess the impacts of the SCIX stream on the DWPF process, one must first select a specific sludge/frit system. Once the sludge/frit system is selected, the impacts of IE-911 to this baseline can be established and evaluated. For this assessment, the Frit 320 –SB4 system as defined by Lilliston (2004) will serve as the baseline flowsheet against which the relative impacts of adding IE-911 will be evaluated. There are obvious advantages and potential disadvantages of selecting the Frit 320 – SB4 system. Advantages include a documented sludge composition and the coincidence of schedules given the spent IE-911 is anticipated to be generated (if implemented) with SB4. The use of Frit 320 is on firm technical ground given it was the frit utilized by Lilliston (2004) during the initial assessments of various washing and blending strategies for SB4. Further, it has been used during assessments of previous sludge batches and has been found to have broad applicability as well as the potential to improve waste throughput for DWPF.

The primary disadvantage of using this specific system is that the projected composition used by Lilliston (2004) is expected to change not only in chemical make-up but in mass as well. Given potential SB4 composition changes, use of Frit 320 may not be "optimal" and therefore its use may establish a biased projected operating window. It should also be noted that Frit 320 may not be optimal (in terms of providing a maximum projected operating window and/or minimizing issues associated with melt rate and/or waste throughput) for the baseline sludge composition reported by Lilliston (2004). In fact, "optimal" frit compositions may differ for a sludge-only flowsheet as compared to a "coupled-operations" flowsheet. Despite these potential disadvantages, the SB4 composition reported by Lilliston (2004) will be used to establish the baseline, sludge-only flowsheet given it is the only documented SB4 composition available and SB4 is expected to coincide with the timing of SCIX, and future sludge batch compositions have even greater uncertainty.

Lilliston (2004) also provides insight into the projected mass for SB4 (237,617 kg on a calcined oxide basis). Given the IE-911 is to be blended with SB4 to assess the impact on DWPF, changes in the actual SB4 mass could result in different projected results. For example, use of a "low" SB4 mass would result in a more significant compositional impact to an overall blended sludge (i.e., SB4 + IE-911). More specifically, the low SB4 mass would not "dilute" the IE-911 as much as a larger SB4 mass. This could drive process control models to over- or under-predict the anticipated impact of IE-911.

Four primary inputs are required to assess the impact on DWPF's CPC and projected operational windows. These inputs are: (1) the SB4 sludge composition, (2) the frit composition, (3) composition of the IE-911 stream, and (4) the nominal process masses and the timing for processing in DWPF, including the sludge and IE-911 stream. These inputs are presented in the following subsections.

### 4.2 SB4 Sludge Composition

Table 12 summarizes the projected SB4 composition as reported by Lilliston (2004). The elemental concentrations provided were converted to an oxide basis (by multiplying by the appropriate gravimetric factor) and normalized.

Table 12. Projected SB4 Composition (calcined oxide basis, wt%) (from Lilliston 2004).

| Oxide                          | SB4    |
|--------------------------------|--------|
| Al <sub>2</sub> O <sub>3</sub> | 21.09  |
| BaO                            | 0.31   |
| CaO                            | 2.35   |
| $Ce_2O_3$                      | 0.33   |
| $Cr_2O_3$                      | 0.36   |
| CuO                            | 0.10   |
| $Fe_2O_3$                      | 29.05  |
| $K_2O$                         | 0.17   |
| $La_2O_3$                      | 0.13   |
| MgO                            | 0.36   |
| MnO                            | 6.55   |
| $Na_2O$                        | 12.96  |
| $Nb_2O_5$                      | 0.00   |
| NiO                            | 8.57   |
| PbO                            | 0.13   |
| $SiO_2$                        | 3.73   |
| $ThO_2$                        | 0.07   |
| $TiO_2$                        | 0.00   |
| $U_3O_8$                       | 13.07  |
| ZnO                            | 0.15   |
| $ZrO_2$                        | 0.52   |
|                                |        |
| Total                          | 100.00 |

### **4.3 Frit Composition**

The nominal Frit 320 composition (with the acceptable tolerance values) is shown in Table 13. It should be noted that the nominal values (with no variation) shown in Table 13 were used in the assessments.

Although Frit 320 is used it should not be considered an optimized frit for any of the systems assessed in this report. Its use in this report is strictly for demonstrating the impact of IE-911 relative to the baseline flowsheet as documented by Lilliston (2004). If negative impacts to the projected operating window result with Frit 320, there is a high probability that strategic glass formulation efforts (via designed frits with an integrated systems approach in mind) could mitigate these impacts and restore the projected operating windows.

Assessments of melt rate for the Frit 320 – SB4 system have not been performed. Prior to implementation of any frit into DWPF, laboratory assessments of melt rate should be made to ensure that what appears attractive on paper (projected operating windows based on model predictions) does not result in a difficult feed to process.

Table 13. Nominal Composition of Frit 320 (with acceptable tolerance ranges).

| Oxide             | wt%          |
|-------------------|--------------|
| $B_2O_3$          | $8 \pm 0.5$  |
| Li <sub>2</sub> O | $8 \pm 0.5$  |
| Na <sub>2</sub> O | $12 \pm 0.5$ |
| SiO <sub>2</sub>  | $72 \pm 1.0$ |
|                   |              |
| Total             | 100          |

### 4.4 Nominal Process Masses and Timing for Incorporation

For this assessment, data from Lilliston (2004) was used to estimate the mass of SB4 oxides, while projections from column modeling described above were used to estimate the mass of IE-911 to be incorporated. Section 4.5 provides additional and more specific information regarding the projected mass of both IE-911 and SB4 as well as the blending strategy used to define an overall sludge composition to support the model-based assessments. Table 14 summarizes the nominal composition of the caustic-washed IE-911 sorbent used in this assessment.

Table 14. Nominal Composition of Caustic-Washed IE-911 Sorbent. (normalized oxide wt%, calcined basis)

| Oxide                          | IE-911 |
|--------------------------------|--------|
| $Al_2O_3$                      | -      |
| BaO                            | -      |
| CaO                            | -      |
| Ce <sub>2</sub> O <sub>3</sub> | -      |
| $Cr_2O_3$                      | 1      |
| CuO                            | 1      |
| $Fe_2O_3$                      | 1      |
| K <sub>2</sub> O               | 1      |
| $La_2O_3$                      | 1      |
| MgO                            | 1      |
| MnO                            | 1      |
| Na <sub>2</sub> O              | 15.15  |
| $Nb_2O_5$                      | 21.11  |
| NiO                            | -      |
| PbO                            | -      |
| $SiO_2$<br>$SO_4^{2-}$         | 17.88  |
| $SO_4^{2-}$                    | -      |
| $ThO_2$                        | -      |
| TiO <sub>2</sub>               | 30.41  |
| $U_3O_8$                       | -      |
| ZnO                            | -      |
| ZrO <sub>2</sub>               | 15.45  |
|                                |        |
| Totals                         | 100.0  |

#### 4.5 Blending Strategy and Assumptions

As previously discussed, the ion exchange operating scenario selected for projecting the quantity of spent IE-911 was using the 0.005 Ci/gal target at 6 gpm flow rate. To obtain an overall "blended" (coupled) sludge composition, the mass of IE-911 (26,786 kg as oxides) was blended with the entire SB4 calcined solids mass (237,617 kg). Figure 15 depicts the blending strategy that forms the basis from which the model-based assessments were made. The "blended" sludge was then coupled with Frit 320 over WL ranges of 25 – 60% resulting in specific glass formulations. The PCCS models (Brown, Postles and Edwards (2002)) were used to predict properties which were ultimately used to classify a glass as "acceptable" (passes all processing criteria) or "not acceptable" (fails one or more processing criteria). The WL interval in which all glasses were deemed "acceptable" determined the projected operating window. A more detailed

<sup>&</sup>lt;sup>1</sup> Various blending and transfer strategies for SB4 have been developed and are being considered. Included in those options is the possibly of two transfers of SB4. If realized, the mass to which CST would be blended may differ depending upon implementation of the SCIX process and integration into the overall SB4 flowsheet.

assessment of this process will be discussed in Sections 5.0 and 6.0. The resulting "blended" sludge composition (total waste oxide mass of 264,403 kg) is presented in Table 15.

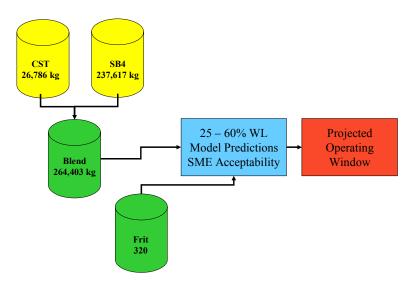


Figure 15. Schematic of SB4 and IE-911 Blending Assumptions

Table 15. Resulting SRAT Product for the IE-911/SB4 Blend (wt% calcined oxide basis)

|                   | IE-911/SB4 |
|-------------------|------------|
| Oxide             | Blend      |
| $Al_2O_3$         | 18.96      |
| BaO               | 0.28       |
| CaO               | 2.11       |
| $Ce_2O_3$         | 0.29       |
| $Cr_2O_3$         | 0.32       |
| CuO               | 0.09       |
| $Fe_2O_3$         | 26.10      |
| K <sub>2</sub> O  | 0.16       |
| $La_2O_3$         | 0.12       |
| MgO               | 0.32       |
| MnO               | 5.88       |
| Na <sub>2</sub> O | 13.18      |
| $Nb_2O_5$         | 2.14       |
| NiO               | 7.70       |
| PbO               | 0.12       |
| SiO <sub>2</sub>  | 5.16       |
| $ThO_2$           | 0.06       |
| TiO <sub>2</sub>  | 3.08       |
| $U_3O_8$          | 11.74      |
| ZnO               | 0.14       |
| ZrO <sub>2</sub>  | 2.03       |
|                   |            |
| Total             | 100.0      |

### 4.6 Impacts to DWPF CPC Processing

The main objectives of the CPC in the DWPF are the destruction of nitrite, reduction of mercury and manganese, neutralization of the base equivalents in the sludge, and adjustment of the slurry rheology to facilitate processing in the melter. This is accomplished by adding formic and nitric acid in the Sludge Receipt and Adjustment Tank (SRAT) and boiling the sludge under reflux. Currently, the amount of acid to be added to each CPC SRAT batch is calculated based on the composition of the sample pulled from the SRAT after sludge transfers from the feed tank. The inputs to the acid calculation include the concentrations of nitrite, manganese, mercury, hydroxide, and inorganic carbon and the slurry volume and density. For this evaluation, it was assumed that none of these components would be present in the SCIX material transferred to Tank 51. At the conclusion of salt solution processing, the IE-911 is washed with water and transferred with water to the grinder, displacing any of these constituents. Therefore the SCIX process would be anticipated to have minimal impact on these parameters, and, thus, no additional calculated acid requirement would be anticipated from the introduction of the SCIX feed. It is recognized that the CST material could return to the hydrogen form during SRAT

processing; however, this chemical change could only be accounted for in the acid calculation if the chemical reaction occurred during the titration determination for hydroxide concentration. In any case, the contribution would be expected to be small compared to the acid demand from SB4 sludge due to the large mass/volume differences.

None of the previous studies with CST showed an increase in acid demand (Lambert and Monson (1998), Daniel 2000, and Koopman and Lambert (2001)). However, inconsistent results were provided on the influence on hydrogen generation during the CPC processing. Lambert and Monson (1998) testing showed increased hydrogen generation in runs containing CST with HM levels of noble metals added to the sludge regardless of the particle size of the CST. The hydrogen peaks came at the start of boiling after CST was added. They also saw significant foaming during their runs. Before the CST was tested in the SRAT run, it was soaked in caustic, dried, and ground as necessary. For this testing, the smallest particle size was 33% >352 um, slightly larger than the SCIX process. Nevertheless, the authors hypothesized that the results of the testing may have been influenced more by some of the input parameters than the actual CST material. The authors recommended additional testing with CST more prototypical of the process flowsheet. Daniel (2000) showed no significant impact on hydrogen generation when lower noble metals levels and loaded CST that was less washed and from a different batch was used. Finally, Koopman and Lambert (2001) tested nominal sludge batch 1b levels of noble metals (110%) and CST loaded with non-radioactive Cs in three CPC runs involving sludge only testing, size-reduced CST (similar to frit particle size) with melter feed, and as-received CST with melter feed. Slightly different sludge and CST loadings were used in the three runs. Slight changes in hydrogen generation were seen between the sludge only and the CST containing SRAT runs. However, the differences were not of practical concern due to the small amounts detected. The size-reduced CST produced slightly more hydrogen and foaming. As with all other streams or any sludge batch proposed for processing in DWPF, a confirmatory study with the sludge simulant and IE-911 should be performed to determine the impact of that material on the particular sludge batch processing.

While achieving the stated objectives is important to meeting the chemical process and glass product constraints, the DWPF must also be concerned with process operations including the ability to sample the material, mix and transfer the material, and meet processing time goals. The DWPF must sample the SRAT receipt material, the SRAT product, the Slurry Mix Evaporator (SME) product, and the Melter Feed Tank (MFT) slurry, as necessary. A Hydragard<sup>®</sup> sampler is used to obtain the representative samples, and it has specific allowable particle size ranges to avoid pluggage: ≤2 wt% at >80 mesh; ≤10 wt% at > 200 mesh. The grinding of spent IE-911 is being performed to meet this specification. Qureshi (1999) performed testing with a CST/water slurry and CST in melter feed slurry. The CST/water slurry testing was performed to determine if DWPF tanks could resuspend CST slurry and to test the impact of agitation in the tanks and pumping with a centrifugal pump on particle size. The melter feed slurry testing was performed at ~40 wt% total solids to determine the Hydragard<sup>®</sup> sampler capability with two different particle size CST materials. The CST/water slurry tests showed problems with mixing and some shearing of the particles, but no problems were experienced with starting and stopping the agitator. In the melter feed testing, the agitator homogeneously mixed the slurry, but Hydragard<sup>®</sup> sampler problems were experienced as evidenced by frit depletion for the size reduced CST and pluggage in the as-received CST

testing. Subsequent Hydragard® testing by Edwards et al. (2000) used a melter feed simulant containing sludge at 26 wt% waste loading and CST at 10 wt% waste loading (both on an oxide basis). The total solids content of the melter feed was either 42 or 46 wt%. Testing at 52 wt% total solids with the CST containing slurry was cancelled since the feed could not be agitated because the yield stress was too high. The two feed streams were evaluated against the baseline melter feed without CST. The CST in this study was "size-reduced" with a maximum size <177 µm. The testing found that the CST did not enhance the enrichment of sludge or the depletion of frit observed for the sludge only case, and the results suggested that differentiation may have been slightly mitigated in the presence of CST. The overall conclusion was that CST behaved similar to sludge in terms of the Hydragard® sampler and the test was not plagued by the plugging problems experienced in earlier testing with larger sized CST. Although the later results were promising, a paper study evaluation should at a minimum be performed to examine the impact of the ground IE-911 from the SCIX process after the process is completely defined and the sludge properties are known. This is necessary due to the numerous parameters that have changed since the testing was performed.

Past SRNL studies have shown that the ability to suspend in solution, mix, and transfer IE-911 depends greatly on the particle size (Hansen et al. (2001), Koopman and Eibling (2000), Edwards et al. (2000), Koopman and Lambert (2001), and Baich 2000). In most cases, the larger-sized CST particles proved to be more difficult and had a greater impact on rheology. For size-reduced CST streams, a well-mixed tank could be obtained even with the significantly increased yield stress. Edwards et al. (2000) attributed this to the comparable consistencies to the sludge-only feed, which implied that once the CST slurries were flowing they behaved similarly. Koopman and Lambert (2001) had difficulties re-suspending the "as-received" CST stream before it was added to the CPC vessels with the sludge feed. They also noted a tendency for the CST to settle in the SRAT and SME during processing. Since these past studies did not focus on the behavior of IE-911 after blending with a sludge slurry in the same fashion as proposed for the current SCIX strategy mixing and pumping studies are recommended to ensure that the process scenario envisioned for Tank 51H will not impact the ability of DWPF to receive or transfer feed. The goal of the studies should be to determine whether the ground IE-911 and sludge mixture:

- can be suspended when dumped in Tank 51H,
- can be resuspended in Tank 51H and as necessary in Tank 40, and
- will impact pumping and mixing (i.e., slurry rheology) in the DWPF CPC vessels.

Finally, the SRAT and the SME are not the time-limiting steps in the DWPF at present. However, the effects on processing time for the introduction of any secondary streams in DWPF must be considered. Based on the proposed SCIX incorporation strategy, no impact on processing time is anticipated. This offers the SCIX an advantage over some of the other salt processing alternatives, which have a large volume of solution associated with their transfers to DWPF.

## 4.7 Approach for Evaluating the Impacts to Glass Properties

Using the available PCCS models, the SCIX stream was assessed in terms of the predicted impacts to the projected operating windows relative to the Frit 320 – SB4 (sludge-only) flowsheet. In this section, the approach or strategy to make such comparisons is presented. It should be noted that the assessments are solely model-based. That is, the operating windows (defined in terms of waste loadings over which acceptable glasses can be made) will be projected using composition – property models that are currently defined in PCCS. No experimental work was performed as a part of this assessment.<sup>2</sup>

Two stages of investigation have been proposed by Peeler and Edwards (2002) to assess various frit/sludge combinations: the Nominal Stage and the Variation Stage. In this study, the Nominal Stage utilizes nominal compositions representing the combination of Frit 320 and the projected sludge compositions (sludge-only and coupled). In general, this stage is used to provide or project the operational windows (in terms of waste loadings allowed) for the nominal compositions considered. It is important to note that during this stage, composition variation in the sludge and/or IE-911 is not accounted for – strictly nominal compositions are considered. Assessments are made using predictions from models currently implemented in the DWPF over the WL interval of interest (25-60 wt%). The primary property predictions assessed include those for liquidus temperature  $(T_L)$ , viscosity  $(\eta)$ , durability (e.g., normalized boron release – NL [B]), the constraints associated with durability (Al<sub>2</sub>O<sub>3</sub> and sum of alkali), and specific solubility limits (e.g., TiO<sub>2</sub>). It should be noted that anion concentrations associated with SB4 were not provided by Lilliston (2004). Therefore, assessments of  $SO_4^{2-}$  solubility as a function of WL were not conducted in this work. Since PCCS has an associated SO<sub>4</sub><sup>2</sup> solubility limit, it is possible that the projected operating windows shown in this report could be altered if  $SO_4^{2-}$ concentrations projected in glass exceed the imposed PCCS limit. It is noted that introduction of IE-911 does not increase the concentration of  $SO_4^{2-}$  (not associated with its composition as shown in Table 14), but does have the potential to dilute the impact of  $SO_4^{2-}$  in SB4.

The impact of the Cs-137 added to each canister from this process is negligible. Summing the total Curies removed at 6 gpm flow rate and 0.005 Ci/gal exit criterion from Table 9 results in 2.2E6 Ci. If this activity is distributed in 442 canisters, it equates to 5.0E3 Ci/canister. At 4.95E-3 watts/Ci, this is 25 watts; versus a DWPF limit of 437 watts (Rios-Armstrong, 2004).

The intent or focus of the Variation Stage (Stage 2) assessment is to gain insight into the robustness of the system with respect to compositional variation. Although an extremely valuable tool, the Variation Stage was not used for this study. All assessments were performed on nominal compositions, since there is no basis for evaluating the variability at this early stage.

 $<sup>^2</sup>$  It is noted that Edwards et al. (1999) and Edwards et al. (2001) did experimentally assess the impact of CST and MST on various glass physical properties including durability (as defined by the PCT), liquidus temperature ( $T_L$  – using isothermal heat treatments), and viscosity. These studies were based on specific flowsheets (HM, Purex, and Blend sludges coupled with unique frits at relatively low waste loadings ( $\sim$ 30%)) and may not be directly applicable to future processing. More specifically, sludge blending and frit development strategies have changed, as well as DWPF has been targeting WLs of > 35%. However, the results of these experimental studies will be referenced in the discussion that follows when warranted in particular to provide some indication of how the model predictions may or may not be applicable.

## 4.8 Measurement Acceptability Region (MAR) Limits Used for Assessments

The glass property predictions assessed in this study included durability (Product Consistency Test [PCT] [ASTM 2002] response in terms of the preliminary glass dissolution estimator ( $\Delta G_P$ ) (Jantzen et al. 1995)), viscosity at 1150 °C ( $\eta_{1150^{\circ}C}$ ),  $T_L$ , and  $Al_2O_3$  and alkali concentrations. Jantzen et al. (1995) and Brown et al. (2001) provide a more detailed discussion on the development of these models. A brief review of the previous experimental work (Edwards et al. (1999) and Edwards et al. (2001)) will provide some insight into the applicability of these models to CST-based glass systems. That is, prior to using the model output as "definitive", one should have a clear understanding of any potential issues associated with applying the models to a compositional region of interest. Given no experimental work was performed as part of this study, one can only use historical information to make this assessment and then use judgment on how that may influence the comparisons made based solely on model predictions for future systems.

With respect to applicability of the durability models, the historical CST/MST results suggest that (in general) the model under-predicted the PCT response as compared to the measured response. That is, the measured PCT responses were greater (i.e., less durable glasses) than model predictions as indicated by their presence above the 95% upper prediction limit. Although unpredictable by the durability model, the glasses were acceptable when compared to the benchmark EA glass. Edwards et al. (2001) provided possible causes for the lack of predictability as being: (1) due to the presence of  $Nb_2O_5$  (not accounted for in the model) and/or (2) the glasses possibly being phase separated. Regardless of the cause, it would appear that model revisions could (or should) be made to ensure predictability. Given no revisions have been made since those assessments, applicability of the model to the system of interest (Frit 320 – SB4) may have similar results – although no experimental work will be performed to confirm this as part of this study. The report also states that niobium is "an element with an unknown impact on glass quality and processing properties" – an issue that is addressed in a paragraph to follow.

The previous work suggests that both the  $T_L$  and viscosity models appear to be "adequate" to cover the compositional ranges of CST-based glasses. That being said, with respect to viscosity, Edwards et al. (1999) indicated that for the Purex based glasses, although the measured viscosities were within the DWPF range of 20-100 Poise, the model, in general, over predicted the measured values. They indicated that "this was not surprising given the fact that the model was not developed for glasses incorporating CST elements". For other CST/MST sludge based systems the viscosity model appeared to predict rather well.

With respect to  $T_L$ , the historical results suggested that the  $T_L$  model was conservative (i.e., over predicted) as compared to the experimentally determined values. It should be pointed out that the measured values were compared to the original  $T_L$  model predictions – not the current  $T_L$  model (Brown et al., 2001) implemented in DWPF. Although an assessment of the current  $T_L$  model predictions could be made relative to the historical data to provide some guidance, such an effort is considered outside the scope of this report.

To summarize, the historical data do raise some concerns regarding the applicability of the PCCS models to CST-based glasses. This concern is reflected in the previous reports via statements regarding the need for model revision or refinements to include terms such as  $Nb_2O_5$  or  $ZrO_2$  given their contributions were not accounted for during the model development efforts. However, to provide guidance to the current program and its objectives, the PCCS models currently implemented in DWPF will be used to make assessments regarding the impact of the CST flowsheet on projected operating windows with an understanding of the potential associated uncertainties. Given no experimental work is performed as part of this study, those uncertainties will remain unknown.

To project operational windows for sludge/frit scenarios of interest, the predicted properties must be assessed relative to established acceptance criteria. Acceptable predicted properties for this assessment are based on satisfying their respective (and most restrictive) Measurement Acceptability Region (MAR) limit values. Brown, Postles, and Edwards (2002) provide a detailed discussion of how the MAR limits are utilized in PCCS. It should be noted that the MAR limits are compositionally dependent for some properties (i.e., will change as a function of glass composition); thus a table can not be shown with "standard" or "set" values. Although the models and acceptance limits are seemingly well-defined, some interesting technical issues result with the introduction of the IE-911 with respect to glass chemistry and model predictions (some of which were identified during the previous experimental assessments). A brief discussion of the primary compositional concerns and potential model validity issues is provided below.

The introduction of significant quantities of TiO<sub>2</sub> from CST could present interesting technical issues associated with the application of the compositional-based models and specific individual "solubility" limits within PCCS. In terms of solubility limits, Lorier and Jantzen (2003) have provided the technical basis for raising the current 1 wt% TiO<sub>2</sub> limit in PCCS to 2 wt% (if needed), although this has not been implemented at DWPF. The primary driver for this technical baseline change was that introduction of TiO<sub>2</sub>-based sorbents could result in the individual TiO<sub>2</sub> solubility limit of 1 wt% being exceeded; thus, WL would be artificially limited or significant impacts could occur to the projected operating windows (assuming no other property prediction restricted access to higher WLs until TiO<sub>2</sub> reached the 1 wt% limit in glass). For the CST-based assessment, the TiO<sub>2</sub> solubility limit was set at 1 wt% (ignoring measurement uncertainties). If this limit restricted access to higher WLs, use of the 2 wt% limit was evaluated to determine the extent to which the projected operating window would benefit. The 1 wt% limit was intentionally used so the need for a higher PCCS limit could be identified for the CST option being considered, i.e., it was used as a flag in the model assessment to identify when the limit needed to be raised. One of the primary drivers for assessing the SCIX IE-911 option was that less IE-911 would be utilized than in previous treatment strategies. Therefore, the amount of TiO<sub>2</sub> added to the glass would be limited – thus the 1 wt% limit was retained to determine if it was adequate, and only relaxed if all other constraints were satisfied. Further, no accounting for titania originating from MCU operation, or uncertainty in the titania in sludge, was included in this assessment, so the use of the 1 wt% limit identifies the need for margin in the titania budget if SCIX and MCU operate concurrently. As previously mentioned, an assessment of the historical CST data to the current model predictions is deemed outside the scope of this report. The current T<sub>L</sub> model will be used to support this assessment without a full understanding of its direct applicability.

The CST sorbent does introduce  $Nb_2O_5$  into the glass. Although  $Nb_2O_5$  can be accounted for in the durability model predictions, its anticipated positive impact on durability is not currently programmed into PCCS; however,  $Nb_2O_5$ 's impact to other properties (such as liquidus temperature and viscosity) is less certain (a statement that is consistent with historical assessments). More specifically, these models do not include a  $Nb_2O_5$  term and therefore predictions of its impact (or lack thereof) cannot be fully addressed. Based on the concentration of  $Nb_2O_5$  in the "blended" SRAT product the impact of  $Nb_2O_5$  on the predicted glass properties is not expected to be significant.

Although extensive models are integrated into the PCCS SME acceptability process for product performance (durability) and melter processing issues, a model for melt rate does not currently exist. Therefore, assessments of melt rate for the Frit 320 – SB4 baseline and the IE-911-based flowsheet can only be made via experimental work – which is not covered under this scope. Melt rate has been a critical factor in supporting the accelerated clean-up mission at DWPF. Prior to implementation of a specific frit and/or introduction of a secondary stream (i.e., IE-911), assessments of melt rate should be made to ensure that what appears attractive on paper (projected operating windows based on model predictions) does not result in a difficult feed to process.

#### 4.9 Nominal Stage Assessments

Table 16 summarizes the MAR-based Nominal Stage assessments. In addition to the MAR-based projected WL interval, the property or single component solubility limit that restricts access to higher WLs is also provided in parentheses. The primary objective is to assess the relative impact of the IE-911 sorbent stream to the projected operating window in relation to the Frit 320 – SB4 baseline.

Table 16. Nominal Stage Assessment Using MAR Criteria

| Option                  | WL range                  |
|-------------------------|---------------------------|
|                         | (limiting property)       |
| Frit 320 – SB4 Baseline | $25 - 30 (T_L)$           |
| Frit 320 – IE-911 – SB4 | $25 - 31 \text{ (TiO}_2)$ |

In the following sections, a more detailed discussion of the projected operating windows is provided for each option. Table B.1 in Appendix B provides a summary of the MAR-based assessments and various predicted glass properties for these systems. The nomenclature used in Appendix B is consistent with that used by Peeler and Edwards (2002), and for a detailed discussion, the reader is referred to that report.

#### 4.10 Frit 320 - SB4 Baseline

For the Frit  $320 - \mathrm{SB4}$  baseline system³, as WL increases the predicted  $T_L$  increases until the predicted  $T_L$  value exceeds the MAR criterion at and above WLs of 31% (see Table B.1 in Appendix B for more details). At 30% WL and below, all property predictions "pass" the SME acceptability process at the MAR. Therefore, the projected operating window for the Frit  $320 - \mathrm{SB4}$  baseline flowsheet is 25 - 30% WL (as shown in Table 16). Although  $T_L$  is the limiting property, another interesting property to evaluate is viscosity. In general, as WL increases, viscosity decreases and does not become a limiting factor until ~59% WL at which the PCCS low viscosity criterion is not met. With respect to frit development efforts, one would view this system as potentially being "non-optimized" as additions of alkali to the frit (relative to Frit 320) could potentially decrease  $T_L$  to allow access to higher WLs. The question then becomes, how much alkali could be added before another property would be challenged. This concept is further explored in Section 4.13.

In support of the main objective of this task, it suffices to say that the Frit 320 –SB4 baseline flowsheet has a projected operating window of 25 - 30%. With this established, the impact of adding IE-911 to the baseline flowsheet can be evaluated.

#### 4.11 Frit 320 - SB4 - IE-911

Based on model predictions (see Appendix B for more details), the projected operating window for the Frit  $320 - \mathrm{SB4} - \mathrm{IE}$ -911 (blended) flowsheet is 25 - 31% WL. At 32% WL, the system becomes  $\mathrm{TiO}_2$  limited (i.e., the  $\mathrm{TiO}_2$  concentration in glass exceeds the 1 wt% MAR limit (after uncertainties are applied) used during the Nominal Stage assessment). If the  $\mathrm{TiO}_2$  limit were increased to 2 wt%,  $\mathrm{TiO}_2$  concentrations in glass would not be a concern over the entire 25 - 60% WL range. With the 2 wt%  $\mathrm{TiO}_2$  limit imposed, the projected operating window would be 25 - 32% WL since the  $\mathrm{T}_L$  MAR is exceeded at 33% WL. At 32% WL, the calculated  $\mathrm{TiO}_2$  concentration is actually 0.986 wt%; while this is not above 1 wt%, the measurement uncertainty imposed by the MAR would prohibit this composition unless the limit was raised.

Regardless of the  $TiO_2$  limit used, the most interesting observation is the fact that addition of IE-911 to SB4 enhances the projected operating window. This observation is somewhat counter intuitive given the presence of both  $TiO_2$  (30.41 wt%) and  $ZrO_2$  (15.45 wt%) in the IE-911 and their anticipated negative impact (i.e., increase in  $T_L$  due to their presence). The fact that the addition of IE-911 lowered the  $T_L$  predictions for a given WL relative to the Frit 320 – SB4 baseline flowsheet suggests that blending IE-911 "dilutes" other troublesome components in SB4 that influence the  $T_L$  prediction.<sup>5</sup> More specifically, since the  $T_L$  model is dependent upon the

<sup>&</sup>lt;sup>3</sup> In Appendix A, this option is referred to as the 320 – Original SB4 Baseline option. Use of "original" implies that subsequent (more recent) SB4 compositions will be assessed, which is covered in Section 7.5.

 $<sup>^4</sup>$  It should be noted that the MAR assessments shown in Appendix B utilize a 2 wt% TiO<sub>2</sub> limit. As previously noted, use of the 1% TiO<sub>2</sub> limit restricts access to WLs of 32% and higher (i.e., the TiO<sub>2</sub> concentration in glass for the Frit 320 – SB4 – CST system is 0.986 wt% which fails the MAR once uncertainties are applied). The use of the 2 wt% limit does provide access to WLs up to 32% (a slight increase in the window size) but predictions of  $T_L$  become limiting at 33% WL.

 $<sup>^5</sup>$  At 30% WL, the Frit 320 – SB4 original baseline  $T_L$  prediction is 996.3°C compared to 955.4°C for the Frit 320 – SB4 – CST system.

concentration of  $TiO_2$ , one could anticipate that the contribution of the IE-911 would have a negative impact on  $T_L$ ; thus, further reducing the upper WL achievable since the Frit 320 – SB4 baseline flowsheet is already  $T_L$  limited. However, the DWPF  $T_L$  prediction is also dependent upon  $Fe_2O_3$ ,  $Cr_2O_3$ , NiO,  $SiO_2$ ,  $ZrO_2$ ,  $Na_2O$ ,  $Li_2O$ , MgO, MnO, CaO,  $K_2O$ , and  $Al_2O_3$  concentrations (Brown et al. 2001) with these oxides having different impacts to the magnitude of the predicted value based on the associated model "coefficients". That is, the relative concentration and the associated "coefficient" ultimately dictate the predicted  $T_L$  value. Therefore,  $TiO_2$  may have a role in determining the  $T_L$  value, but may not be the primary contributor given its concentration and "coefficient" product. Therefore, the increased  $TiO_2$  concentration in the blended sludge resulting from the IE-911 addition to SB4 appears to be countered by a dilution effect of other  $T_L$  model contributors resulting in a net decrease in  $T_L$ . In addition to the "dilution" effect, the presence of  $Na_2O$  (15.15 wt%) in IE-911 may also help to reduce the  $T_L$  predictions.

A primary concern with the addition of CST was the  $TiO_2$  concentration and its impact to  $T_L$ , model applicability (in terms of oxide ranges over which the model was developed), and/or the potential to exceed the individual  $TiO_2$  solubility limit. Concern regarding the individual solubility limit was one of the drivers for the report issued by Lorier and Jantzen (2003) which provides justification for raising the  $TiO_2$  solubility limit from 1 wt% to 2 wt% (in glass). As previously noted, issues with the 1 wt%  $TiO_2$  solubility limit are encountered at 32% WL. With respect to the individual solubility limit, the 2%  $TiO_2$  limit (as proposed by Lorier and Jantzen (2003)) is not exceeded over the entire WL interval of interest (25 – 60%).

With respect to  $T_L$  model applicability for this system, the current model was developed over a  $TiO_2$  range of 0 to  $\sim$ 2 wt% (which formed the basis for the decision by Lorier and Jantzen (2003) to raise the limit, if necessary). Other oxides of interest that IE-911 brings to the system include  $ZrO_2$  and  $Nb_2O_5$ . Although the nominal  $ZrO_2$  concentration in the blended sludge is 2.03 wt%, at the upper WL of 32%,  $ZrO_2$  concentrations in glass would be  $\sim$ 0.65 wt%. The  $T_L$  model was developed over a  $ZrO_2$  range of 0.005 to 0.97 wt% - therefore model applicability for  $ZrO_2$  is not an issue. With respect to  $Nb_2O_5$ , this component is not associated with the current  $T_L$  model and therefore its impact is not known. Although unknown, given the nominal  $Nb_2O_5$  concentration in the blended sludge is 2.14 wt%, at WLs of 30 and 32% WL, the projected  $Nb_2O_5$  concentration in glass would be 0.64 and 0.68 wt%, respectively. These concentrations should not significantly impact  $T_L$  – an assumption that must be confirmed via experimental studies. However, as previously mentioned, there has been no formal assessment of model predictions versus actual measurements.

Although no formal assessment of melt rate (via experimental study) was made, literature suggests that the presence of TiO<sub>2</sub> can have a detrimental effect on melt rate (Plodinec 1979, 1980). It should be noted that this latter statement is qualitative in nature and, until quantified for the specific system(s) of interest, should be used with caution (i.e., the option should not be withdrawn based on circumstantial evidence of the presence of relatively high TiO<sub>2</sub> concentrations). The impact of IE-911 on melt rate should be assessed if this process is further

considered.<sup>6</sup> Based on historical results, systems with higher alkali content (or lower viscosities) have generally been characterized by enhanced melt rates. Assuming that trend holds for these systems, one would expect essentially no difference (ignoring the potential negative impacts of TiO<sub>2</sub>) between the Frit 320 – SB4 baseline with or without IE-911. The viscosity and sum of alkali contents for the baseline with and without IE-911 (at 30% WL) are 61.0 Poise versus 60.2 Poise and 18.0 versus 17.9 wt%, respectively.

#### 4.12 DWPF Canister Impact

projected operating window.

In this section, an assessment of the impact of processing IE-911 with SB4 on the number of DWPF canisters is made. That is, what is the impact of adding IE-911 to SB4 (under the assumed blending scenario and masses) on the number of canisters that DWPF would produce relative to the baseline flowsheet? To address this question the following assumptions will be made:

- a DWPF canister holds 4000 lbs of glass,
- the +2% increase in WL (given implementation of the 2 wt% TiO<sub>2</sub> limit) is observed, on average, for all WLs, and
- DWPF would target the maximum WL obtained based on the model assessment (even though waste throughput may not be optimized at the maximum WL).

Table 17 summarizes the canister count impact to DWPF with the addition of IE-911. First consider the "sludge-only" flowsheet (i.e., Frit 320 – SB4). Lilliston (2004) projected the SB4 mass to be 237,617 kg (or 523,856 lbs). Assuming DWPF processed the "sludge-only" flowsheet at 30% WL, the total number of canisters produced would be 437. Based solely on the mass of IE-911 to be processed (59,053 lbs) and a 30% WL for glass containing IE-911 in the DWPF canisters, an additional 50 canisters would be required. If one were to assume that IE-911 had no impact on the projected operating window (i.e., the maximum WL processed would be 30% WL), then a total of 487 canisters would be required to immobilize the "coupled" flowsheet case. However, the addition of IE-911 has a "positive impact" on the projected WL (allowing a 32% WL to be targeted instead of a 30% WL), therefore only 456 canisters would be required. The actual projected difference in the number of canisters between the "sludge-only" baseline and the "enhanced" IE-911 flowsheet is 19 canisters.

<sup>&</sup>lt;sup>6</sup> Experimental assessments of melt rate or waste throughput are not evaluated in this report. The reader should be aware that the melt rate program is a critical component of the integrated glass formulation strategy as it ensures that what appears attractive on paper (in terms of model-based WL ranges) does not result in a difficult feed to process. In fact, historical information indicates that the maximum waste throughput is not obtained at the maximum WL but at some lower, intermediate value within the

<sup>&</sup>lt;sup>7</sup> The number of canisters is calculated as: ((lbs of sludge) / (lbs of glass per canister)) / (WL). A partial canister is considered a full canister.

**Table 17. Impact to DWPF Canister Count** 

|    | Sludge-<br>Only | IE-911-<br>Only |           |           |             |
|----|-----------------|-----------------|-----------|-----------|-------------|
|    |                 |                 | N. IE 011 | TE 011    | 01 1 0 1    |
|    | 523,856 lbs     | 59,053 lbs      | No IE-911 | IE-911    | Sludge-Only |
|    |                 |                 | Impact    | +2% WL    | Versus 2%   |
|    |                 |                 |           | Impact    | Impact      |
| WL | # of            | # of            | # of      | # of      | Δ Canisters |
|    | canisters       | canisters       | canisters | canisters |             |
| 30 | 437             | 50              | 487       | 456       | 19          |
| 31 | 423             | 48              | 471       | 442       | 19          |

Obviously adding more mass to the baseline flowsheet with the addition of 59,053 lbs of IE-911 will generate an increase in the discrete number of canisters (assuming all other factors equal), but the enhanced operating window (from 30 to 32% WL) obtained by the addition of IE-911 partially offsets the difference in the number of canisters needed. As was previously noted, time of processing (i.e., melt rate) is not factored into this equation. That is, if IE-911 had a significant negative impact on melt rate, processing time to fill the canisters would be extended although the number of canisters would remain the same.

The results indicating that IE-911 is advantageous to the SB4 system are encouraging. However, there are potentially three major issues that could be artificially enhancing its impact on the projected operating windows. These issues are: (1) the baseline system was not "optimized", (2) the mass of SB4 to which the IE-911 is blended could be larger than the 234,617 kgs reported by Lilliston (2004), and/or (3) the composition of the SB4 to which the IE-911 is blended could be significantly different than the original baseline composition provided by Lilliston (2004). These issues are addressed in the next two sections.

#### 4.13 Optimizing the "SB4" Baseline Flowsheet

As mentioned in the previous section, the use of Frit 320 with SB4 may not be optimal with respect to the size of the projected operating window. More specifically, alternative frit compositions could be developed which not only increase the projected operating window size but also mitigate (or minimize) the positive impact of IE-911 once blended. To address this issue, a limited "paper" scoping study was performed to determine if an alternative frit could be developed to increase the operating window size. As a result of this study, Frit 440 was defined (see Table 18 for the nominal composition). Compared to Frit 320, the Na<sub>2</sub>O concentration has increased from 12% to 20% which should lower T<sub>L</sub> and potentially allow for higher WLs to be achieved (given the Frit 320 – SB4 baseline was T<sub>L</sub> limited). The model-based predictions of the Frit 440 – SB4 system result in a projected operating window of 25 – 32% WL (a 2% increase over the Frit 320 – SB4 baseline without IE-911). Appendix C provides the MAR based assessments and various property predictions for the alternative cases considered in this report. The Frit 440-based system is still T<sub>L</sub> limited at WLs of 33% or greater which suggests further increases in the Na<sub>2</sub>O content of the frit may continue to push toward higher WLs. However,

additional alkali increases to the frit drastically reduced the predicted durability. Although Frit 440 may not be "optimized" for the nominal SB4 sludge-only composition, the effect of frit development to improve the projected operating window has been demonstrated. A follow-up assessment was performed to determine if the addition of IE-911 has the same beneficial effect in terms of extending the upper WL achieved for the Frit 440 – SB4 system.

**Table 18. Nominal Composition of Frit 440** 

| Oxide             | wt%   |
|-------------------|-------|
| $B_2O_3$          | 7.7   |
| Li <sub>2</sub> O | 3.0   |
| Na <sub>2</sub> O | 20.0  |
| SiO <sub>2</sub>  | 69.3  |
|                   |       |
| Total             | 100.0 |

Table 19 summarizes the projected operating windows for the Frit  $440 - \mathrm{SB4}$  baseline with and without IE-911. As noted above, the baseline without IE-911 has a projected operating window of 25 - 32% WL (with the system being  $T_L$  limited at higher WLs). Once the IE-911 is blended with SB4 (using the same masses for both as was done with the Frit 320 systems), the projected operating window is 25 - 34% with the increased  $TiO_2$  limit. Again, a 2% increase in the operating window results with the addition of the IE-911 stream. The system is  $T_L$  limited at WLs of 35% and higher.

**Table 19. Projected Operating Windows for Frit 440 - SB4 Systems** 

| Option          | Frit 440        |
|-----------------|-----------------|
| SB4             | $25 - 32 (T_L)$ |
| SB4 with IE-911 | $25 - 34 (T_L)$ |

#### 4.14 Impact of the SB4 Mass and/or Composition

In this section, the impact of IE-911 on the projected operating windows is assessed based on a significant change in the SB4 mass and composition. This assessment is based on speculation that the mass of SB4 may actually be much higher than estimated by Lilliston (2004), and the possibility of significantly different SB4 composition. Although use of the low SB4 mass would be conservative with respect to the potential negative impacts of TiO<sub>2</sub> on DWPF (i.e., the TiO<sub>2</sub> would be more concentrated when blended with a smaller SB4 mass), it may not be conservative with respect to the demonstrated "beneficial" impacts of IE-911 on the projected operating windows. More specifically, if the same mass of IE-911 (59,053 lbs) were blended in a larger mass of SB4, would the "beneficial" effects of IE-911 be "diluted?" To address this issue, more recent (yet still preliminary) compositional projections of SB4 were obtained. The SB4-only

option assumes there will be no heel of SB3 blended with SB4. The 1100 and 1200 equivalent canister options account for varying SB3 heel masses based on different SB3 canister production goals. These compositions and projected masses (calcine oxide basis in kg) are summarized in Table 20.

Table 20. Revised SB4 Compositions and Masses<sup>8</sup>

|                                | 1100 E   | uivalent | 1200 Ea  | uivalent | SR4-     | Only    |
|--------------------------------|----------|----------|----------|----------|----------|---------|
|                                | 1        | ister    |          | ister    |          |         |
| Mass                           | 458515.1 |          | 465556.0 |          | 393,093  |         |
| (kg)                           |          |          |          |          | ŕ        |         |
|                                | 1100     | 1100/CST | 1200     | 1200/CST | SB4 only | SB4/CST |
| $Al_2O_3$                      | 23.47    | 22.17    | 24.78    | 23.43    | 29.84    | 27.94   |
| BaO                            | 0.17     | 0.16     | 0.17     | 0.16     | 0.18     | 0.17    |
| CaO                            | 1.79     | 1.69     | 1.52     | 1.44     | 0.59     | 0.56    |
| Ce <sub>2</sub> O <sub>3</sub> | 0.21     | 0.20     | 0.21     | 0.20     | 0.18     | 0.17    |
| Cr <sub>2</sub> O <sub>3</sub> | 0.26     | 0.25     | 0.26     | 0.25     | 0.27     | 0.26    |
| CuO                            | 0.09     | 0.08     | 0.08     | 0.08     | 0.08     | 0.07    |
| Fe <sub>2</sub> O <sub>3</sub> | 26.92    | 25.44    | 25.23    | 23.86    | 19.59    | 18.34   |
| K <sub>2</sub> O               | 1.06     | 1.00     | 1.22     | 1.16     | 1.84     | 1.72    |
| La <sub>2</sub> O <sub>3</sub> | 0.10     | 0.10     | 0.10     | 0.09     | 0.08     | 0.07    |
| MgO                            | 2.01     | 1.90     | 1.64     | 1.55     | 0.34     | 0.32    |
| MnO                            | 6.04     | 5.71     | 5.79     | 5.48     | 4.92     | 4.61    |
| Na <sub>2</sub> O              | 21.03    | 20.71    | 22.23    | 21.85    | 25.38    | 24.72   |
| $Nb_2O_5$                      | 0.00     | 1.16     | 0.00     | 1.15     | 0.00     | 1.35    |
| NiO                            | 3.85     | 3.63     | 4.22     | 3.99     | 5.63     | 5.27    |
| PbO                            | 0.09     | 0.09     | 0.08     | 0.07     | 0.04     | 0.04    |
| SiO <sub>2</sub>               | 2.83     | 3.66     | 2.71     | 3.54     | 2.31     | 3.31    |
| ThO <sub>2</sub>               | 0.04     | 0.03     | 0.04     | 0.03     | 0.04     | 0.04    |
| TiO <sub>2</sub>               | 0.02     | 1.70     | 0.02     | 1.67     | 0.01     | 1.95    |
| $U_3O_8$                       | 9.60     | 9.07     | 9.28     | 8.78     | 8.26     | 7.73    |
| ZnO                            | 0.13     | 0.13     | 0.13     | 0.12     | 0.11     | 0.10    |
| ZrO <sub>2</sub>               | 0.28     | 1.12     | 0.28     | 1.10     | 0.30     | 1.27    |

These more recent SB4 compositions were coupled with Frit 320, Frit 418, and Frit 440 to assess the projected operating windows with and without IE-911. The results of the model based assessments are shown in Table 21. In general terms, three observations will be highlighted with respect to these data. First, frits that provide operating windows for certain SB4 composition views may not be viable with other compositional estimates. For example, Frit 440 was developed specifically for the initial SB4 composition provided by Lilliston (2004) to increase the operating window relative to Frit 320 (see Section 4.13). Although successful with the initial composition, its use with the alternative or revised SB4 compositions does not result in adequate

<sup>&</sup>lt;sup>8</sup> For comparison purposes, the mass of the initial (or original) SB4 was 237,617 kg as discussed in Section 4.5.

operational windows for DWPF. With respect to the impact of IE-911 to the Frit 440-based, revised SB4 compositional systems, it is difficult to demonstrate the "beneficial" effects given the "sludge-only" flowsheets do not have operating windows. It is interesting to note that the addition of IE-911 to the 1100 Equivalent canister option transitions the projected operation window from non-existent ("sludge-only") to a 46-47% window (with IE-911). Although this small operating window is not practical from a DWPF perspective, it demonstrates the positive effects of IE-911. Use of Frit 320 and Frit 418 with the revised SB4 compositions results in significantly larger operating windows relative to the original SB4 composition. In general, the projected operating windows for these systems range from 25% up to 40-45% WL. The key point is that frit development efforts can establish operating windows for specific waste streams that provide operational flexibility to DWPF.

Table 21. Projected Operating Windows for Various SB4 Systems

| h                         |          |          |          |
|---------------------------|----------|----------|----------|
|                           | Frit 320 | Frit 418 | Frit 440 |
| SB4 (per Lilliston)*      | 25 - 30  | -        | 25 - 32  |
| SB4 (per Lilliston) + CST | 25 - 32  | -        | 25 - 34  |
|                           |          |          |          |
| SB4 revised mass/comp**   | 25 - 45  | 25 – 41  | -        |
| SB4 revised with IE-911   | 25 – 46  | 25 – 43  | -        |
|                           |          |          |          |
| 1100 Equivalent Cans      | 25 - 43  | 25 – 40  | -        |
| 1100 Equivalent Cans      | 25 - 45  | 25 – 41  | 46 – 47  |
| with IE-911               |          |          |          |
|                           |          |          |          |
| 1200 Equivalent Cans      | 25 - 44  | 25 – 40  | -        |
| 1200 Equivalent Cans      | 25 – 45  | 25 – 41  | -        |
| with IE-911               |          |          |          |

<sup>\*</sup>SB4 (per Lilliston 2004) is the original composition and blending strategy in Section 4.11-4.12

The second major point to make, and probably the more significant with respect to the objectives of this task, is the fact that the addition of IE-911 to each of the revised "sludge only" compositional view results in an increase in the projected operating window. Typically, a 1 – 2% increase in the operating window is observed based on model predictions. This observation is consistent with the results of the initial Frit 320 – SB4 system (as discussed in Sections 4.10 and 4.11). These results indicate that the "beneficial" impact of IE-911 is "independent" of the (a) mass of SB4 (within the bounds assessed in this study) and (b) the composition of the sludge/frit system. In terms of the SB4 mass effects, the hypothesis that the "beneficial" effects of IE-911 were based on the inability of the low SB4 mass to dilute the IE-911 was not realized. Again, enhanced operating windows resulted for all four SB4 masses and compositions used in

<sup>\*\*</sup>SB4 revised mass/composition is the most recent estimates of SB4, with no heel of SB3

 $<sup>^9</sup>$  A "-" is used to denoted those systems in which property predictions restrict assess to any WL over the entire 25 - 60% WL range (i.e., no window).

this assessment. The percentage increase as a result of the IE-911 was slightly dependent on the SB4 composition and mass as well as the frit.

A case of potential interest that was not addressed in this study, is the option of using the smaller mass of IE-911 (44,290 lbs or 20,090 kg) as a result of the 0.08 Ci/gal option. Given the unanticipated positive results of IE-911, the question that comes to mind is: "Would the use of a lower mass of IE-911 minimize the positive impacts previously observed?" Obviously there may be several permutations that have not been addressed, but based on the results of this study, it appears that the IE-911 would not have a negative impact on the SB4 system, but actually may enhance its performance with respect to operational window size. This latter statement does not include assessment of melt rate and does not address the concept of targeting a WL that optimizes waste throughput.

#### 4.15 Impact of IE-911 on DWPF Canister Production with the Revised SB4 Compositions

As was performed in Section 4.12, an assessment of the impact of processing IE-911 with the revised SB4 composition and alternative frits is made in this section. The assumptions made in Section 4.12 were used to support this assessment.

Tables 22 through 24 summarize the canister count impact to DWPF with the addition of CST for the most recent SB4-only, 1100 Equivalent Canister, and 1200 Equivalent Canister options, respectively. When considering the sludge-only cases, the number of canisters produced increases as the mass of SB4 increases for a given WL. Again, this is strictly based on an increased mass of sludge to immobilize. First consider the SB4-only case at 30% WL. The number of cans to immobilize the 866,622 lbs of sludge is 723. Given the mass of CST has not changed from the previous canister impact assessment, 50 canisters would be required to immobilize CST only. With the 2% WL enhancement, the projected DWPF operating window would be 32%. The DWPF sludge and CST waste being processed at this higher WL requires only 724 canisters – only 1 more than the SB4 waste alone at the lower (30%) WL. At a targeted WL, the number of canisters does increase with the addition of the CST mass, but the enhanced operating window obtained significantly offsets the difference in the number of canisters needed relative to a "no impact" case. Comparable calculations were performed for the 1100 and 1200 Equivalent Canisters options as well.

As the mass of SB4 increases, the general trend is to reduce the number of additional canisters needed and, in some cases, the number of canisters is actually less that the sludge-only flowsheet even with the increased mass from IE-911. As previously noted, the time of processing (i.e., melt rate) is not factored into this equation. That is, if IE-911 had a significantly negative impact on melt rate, processing time to fill the canisters would be extended although the number of canisters would remain the same.

<sup>&</sup>lt;sup>10</sup> It should be noted that a 2% enhancement is used to assess the impact to canister totals for all three SB4 blending scenarios. Use of the 2% enhancement may not be directly applicable for some options being considered (i.e., 1100 canister option with Frit 418 shows only a 1% enhancement – see Table 4-6). However, use of the 2% enhancement does serve as a general guide given the flowsheets have not been optimized. Tables 4-12 through 4-14 also provide a "worst-case" scenario in terms of canister impacts (i.e., at 30% WL the increase in the number of canisters would be 50 if CST has no "positive impact").

Table 22. Impact to DWPF Canister Count Based on the SB4-Only Revised Composition and Mass

|    | SB4-Only    | IE-911-    |           |           |             |
|----|-------------|------------|-----------|-----------|-------------|
|    | _           | Only       |           |           |             |
|    | 866,622 lbs | 59,053 lbs | No IE-911 | IE-911 +  | Sludge-Only |
|    |             |            | Impact    | 2% WL     | Versus 2%   |
|    |             |            |           | Increase  | Impact      |
| WL | # of        | # of       | # of      | # of      | Δ Canisters |
|    | canisters   | canisters  | canisters | canisters |             |
| 30 | 723         | 50         | 773       | 724       | 1           |
| 35 | 620         | 43         | 663       | 626       | 6           |
| 40 | 542         | 37         | 579       | 551       | 9           |

Table 23. Impact to DWPF Canister Count Based on the 1100 Equivalent Canister Option

|    | Sludge-   | IE-911-    |           |           |                    |
|----|-----------|------------|-----------|-----------|--------------------|
|    | Only      | Only       |           |           |                    |
|    | 1,101,853 | 59,053 lbs | No IE-911 | IE-911    | Sludge-Only        |
|    | lbs       |            | Impact    | +2% WL    | Versus 2%          |
|    |           |            |           | Increase  | Impact             |
| WL | # of      | # of       | # of      | # of      | $\Delta$ Canisters |
|    | canisters | canisters  | canisters | canisters |                    |
| 30 | 843       | 50         | 893       | 836       | -7                 |
| 35 | 723       | 43         | 766       | 723       | 0                  |
| 40 | 632       | 37         | 669       | 637       | 5                  |

Table 24. Impact to DWPF Canister Count Based on the 1200 Equivalent Canister Option

|    | Sludge-   | IE-911-    |           |           |                    |
|----|-----------|------------|-----------|-----------|--------------------|
|    | Only      | Only       |           |           |                    |
|    | 1,026,375 | 59,053 lbs | No IE-911 | IE-911 +  | Sludge-Only        |
|    | lbs       |            | Impact    | 2% WL     | Versus 2%          |
|    |           |            |           | Increase  | Impact             |
| WL | # of      | # of       | # of      | # of      | $\Delta$ Canisters |
|    | canisters | canisters  | canisters | canisters |                    |
| 30 | 856       | 50         | 906       | 848       | -8                 |
| 35 | 734       | 43         | 777       | 734       | 0                  |
| 40 | 642       | 37         | 679       | 647       | 5                  |

## 5.0 System Impacts

#### 5.1 Saltstone

The quantity of salt solution that must be dispositioned as Saltstone could be greatly reduced by this process. In the baseline (Mahoney and d'Entremont, 2004), the total quantity of liquid sent to Saltstone is 5.1 million gallons for Batches 4, 5, 6, and 8. For the SCIX as described, it totals 3.2 million gallons. The difference of 1.9 million gallons of liquid is due to a combination of factors, and represents an estimated cost avoidance of \$7.6 million in making Saltstone (Sethi, Liutkus, and Nash 1997). The sodium content in the planning baseline is much lower than in the SCIX process, due to the low molarity of Recycle waste, and process requirements of MCU. The MCU operates most efficiently with a feed solution sodium molarity of around 6.4 M [Na<sup>+</sup>], and chemical reagent additions within MCU and ARP further reduce the concentration. The resulting sodium molarity for Batches 4, 5, 6, and 8 are as low as 3.2 M [Na<sup>+</sup>], slightly below the WAC for Saltstone of 3.5 to 7.0 M [Na<sup>+</sup>]. As presented here, the SCIX is expected to be within 6.44 to 7.0 M [Na<sup>+</sup>]. It is anticipated that any process control testing needed for incorporation of SCIX effluent would be routine confirmatory tests since the salt solution is expected to be within the current WAC range (Chandler, 2004), other than Cs-137 content. These benefits assume that the DWPF Recycle waste stored in Type IV tanks can be diverted to another disposal path, either for dissolution of salt solution or evaporated.

#### 5.2 Tank Farms

If the proposed operating conditions and schedules can be met, it is possible that free space in the Type III waste tanks could become available earlier. The principal reason for this is related to the reduction in the volume of liquid dispositioned in Saltstone. Since there is 1.9 million gallons less liquid to be disposed (which is mostly Type IV waste or process additions), and the Saltstone processing rate is fixed, the salt solution in Type III tanks may be disposed at a faster rate. To fully evaluate the possible improvement in tank space, a SpaceMan Plus<sup>™</sup> run would be needed so that other parameters can be included, such as the impact on other tank transfers. Two key factors in the achievable processing rate are the allowable effluent activity level and the ability of the rotary microfilter to supply filtered feed solution. At an effluent activity of 0.08 Ci/gal, the column can operate at 15 gpm with a reasonable efficiency. To reach 0.005 Ci/gal at 15 gpm, the efficiency drops by 40%, i.e., 28 columns of IE-911 are needed, vs. 20 at 6 gpm. The rotary microfilter is under development, and its performance has not been fully demonstrated, so projections of flow rate are tenuous.

Equipment for pretreatment of the IE-911 is being developed as part of the design of the SCIX system. The material must be wetted and washed with inhibited water prior to transfer into the column, and equipment and procedures would be needed for implementation.

The conceptual design of the grinder is being tested in SRNL to ensure that the system performs as planned and to estimate the grinding cycle time. Testing includes both a less expensive surrogate zeolite material and a partial batch of IE-911. The research objectives also include examining the wear on the grinder components to estimate lifetime. Results will be published in an upcoming report entitled "Confirmation of Small Column Ion Exchange Crystalline Silicotitanate (CST) Grinder Configuration and Estimation of Treatment Cycle".

The recent redesign of the SCIX was to reduce the weight loading on the tank top. In the prior design, a separate support structure was needed to distribute the weight of the column and grinder modules off of the tank top. The reduced size allows for a "doughnut" of shielding around the valves and pipes in each module, eliminating the need for the support structure. A tank top loading calculation has recently been completed, confirming that Tank 51H can accommodate the weight (McCabe and Phillips, 2004)

A distributed control system would be needed to operate the SCIX, and is being developed by ORNL as part of the project. Other than recharging the column with fresh IE-911, the system is designed to operate remotely.

Safety of the SCIX system was evaluated in a Consolidated Hazards Analysis (Knight and Nguyen, 2004). Design of the system was modified to accommodate the outcome of the evaluation. A strategy and schedule for requesting and obtaining regulatory approval for implementing this system has not been developed.

### **5.3 DWPF CPC Processing**

The three main issues addressed in this report regarding the CPC were the potential impacts of added IE-911 on: (1) the acid addition strategy (and potential hydrogen generation), (2) sampling, pumping, and mixing requirements, and (3) processing times. With respect to the acid addition strategy, the SCIX process is anticipated to have minimal impact. No significant additional acid requirement would be anticipated from the introduction of this stream. Previous studies with CST did not show an increase in acid demand and provided inconsistent results on the influence on hydrogen generation during the CPC processing (Lambert and Monson (1998), Daniel (2000), and Koopman and Lambert, (2001)). However, the impact is anticipated to be negligible. Simulant studies with CST material treated to and at the expected concentration in sludge are recommended to ensure that IE-911 has minimal impact on the CPC processing.

Introduction of IE-911 does pose potential issues regarding sampling, pumping, and mixing. A Hydragard® sampler is used to obtain the samples, and it has specific particle size specifications for the samples to avoid pluggage. The SCIX flowsheet includes a grinding process to meet this specification, and previous Hydragard® testing at this particle size indicated that sampling was not an issue (Edwards et al., 2000). The applicability of the results from the 2000 testing should be judged once the final SCIX flowsheet is defined (i.e., CST loading, sludge loading in the DWPF, etc.). Additional testing with a sludge simulant containing the IE-911 and a system representative of the Hydragard® sampler may be warranted to ensure that pluggage will not occur. The incorporation of the IE-911 may have an impact on slurry rheology, which could impact the ability to transfer and mix the material. Slurry rheology has been shown to be dependent on the sludge composition and has changed with each sludge batch. Furthermore, the proposed addition strategy is different than previous testing. Therefore, mixing and pumping studies are recommended to address potential suspension and rheology issues for the particular system in which the material is added.

Finally, SRAT and SME processing are not the time-limiting steps in the DWPF at present. Based on the proposed SCIX incorporation strategy, no impact on processing time is anticipated.

This offers the SCIX an advantage over some of the other salt processing alternatives, which have a large volume of solution associated with their transfers to DWPF.

#### 5.4 DWPF Projected Operating Windows and Impact to Canister Count

The results of this study indicate that the addition of IE-911 to SB4 (based on the masses and compositional views assessed) has a positive effect on the model-based projected operating windows. More specifically, for all the options evaluated, IE-911 increased the projected operating windows by approximately 2 WL%. This observation was somewhat counter intuitive given the presence of both  $TiO_2$  and  $ZrO_2$  in the IE-911 and their anticipated negative impact. The fact that the addition of IE-911 lowered the  $T_L$  predictions for a given WL relative to the "sludge-only" flowsheets suggests that blending IE-911 "dilutes" other troublesome components in SB4 that influence the  $T_L$  prediction. It should also be mentioned that the  $Na_2O$  contribution from IE-911 may also lower  $T_L$  predictions. The 2 WL% increase was observed for different SB4 compositions, masses, and frit compositions. The projected maximum concentrations of  $TiO_2$  and  $ZrO_2$  (in glass) do not cause concern for either individual solubility limits or  $T_L$  model applicability.

With respect to the impact to DWPF canister count, the results were also encouraging. The positive impact of IE-911 (i.e., potential WL increase) offsets the number of additional canisters expected for the added mass assuming no impact of IE-911 on the operating window. The reduction in the number of canisters was dependent upon the mass of SB4 and the targeted WL. For some cases, the number of canisters was actually reduced by the addition of IE-911 relative to its counterpart "sludge-only" system.

There were some outstanding issues identified during this review. Section 6.0 summarizes these issues.

#### 6.0 Recommendations

This evaluation is an attempt to estimate the system impacts for implementation of SCIX at SRS. There are many assumptions which cannot be immediately confirmed. The waste processing baseline strategy needs to be finalized before more definitive comparisons can be made.

Completion of the design, construction, and testing of the full-scale system, as planned by ORNL, would be needed before implementation. Some details of the system operation can only be determined by demonstration at full-scale, such as the sluicing of IE-911 from the column to the grinder, grinding cycle time, and cumulative pressure loss.

A SpaceMan Plus TM run that incorporates the SCIX is needed to verify the many assumptions used in this evaluation. It is likely that conditions exist that would prohibit incorporation of the SCIX as shown, but most of these probably have workable solutions; for example, since the proposed system dispositions Type III wastes earlier, the transfer lines are not projected to be available when needed to meet this earlier schedule, but it is possible they could be made available. Similarly, tank space for dissolution may be an issue, as well as sampling and

analysis time. There are no known unworkable impediments to this proposed implementation plan.

Regulatory approval for implementing this system has not been requested as it is not an approved project. Also, the schedule for installation of the SCIX has not been fully evaluated, and is tenuous.

Based on the limited assessments performed in this study, which represent a much smaller subset of the traditional impact assessment that is performed by the Closure Business Unit for a new sludge batch or stream to be processed in the DWPF, the IE-911 option being considered is plausible from a DWPF CPC and glass formulation perspective. However, as in a traditional impact assessment, various items were identified that would require further study before all risks would be considered minimized. In many cases, similar studies were performed in the past with CST to determine the risk, but those studies were performed on CST that was of a different composition (due to treatment method) and particle size, assumed a different CST, sludge, and solids loading, and used a sludge simulant that may not be representative of current or future sludge rheology. The open issues are outlined below:

- (1) Demonstrate process-ability of the IE-911 stream with simulant studies
  - with respect to the CPC, issues associated with rheology (mixing and pumping), anti-foam effectiveness, and H<sub>2</sub> generation are of most interest, while impacts to sampling should be able to be assessed based on the results of the mixing and pumping testing
  - with respect to the melter, issues associated with melt rate and cold cap behavior are of interest to reduce the risk that what appears attractive on paper (based on model-based predictions) does not result in a difficult feed to process
- (2) Perform frit development activities to "optimize" the flowsheet with respect to projected operating windows and melt rate (either as an independent study or as part of sludge batch qualification for the sludge batch in which the material is to be incorporated)
  - of particular interest are
    - a. the impact of IE-911 on melt rate,
    - b. the potential need for a  $Nb_2O_5$  term in the PCCS models (in particular the  $T_L$  and/or viscosity model), and
    - c. the need to address potential model applicability issues for select process and/or product quality related properties.

## 7.0 Acknowledgements

The authors wish to gratefully acknowledge the financial support of the U.S. Department of Energy, Office of Cleanup Technologies, and to express their appreciation to the following individuals who made this work possible:

Joe Walker, ORNL Doug Walker, SRNL Chet Miller, U.S. Department of Energy, EM-21
Harry Harmon, PNNL
Patricia Suggs, U.S. Department of Energy – Savannah River
Sam Fink, SRNL
Paul d'Entremont, SRS
Mark Hopkins, SRS
Tommy Caldwell, SRS

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## Appendix A

## VERSE Input: Design 6 with Batch 4/5 Diluted feed stream

```
Design 6, IE-911, L=13ft, D=26.6in, V=375Gal, F=15gpm, T=30C
1 component (Cs) isotherm (Batch 4 Diluted)
1, 50, 3, 6
                                  ncomp, nelem, ncol-bed, ncol-part
FCWNA
                                  isotherm, axial-disp, film-coef, surf-diff, BC-col FCUNA
NNNNN
                                  input-only, perfusable, feed-equil, datafile.yio
                                  comp-conc units
396.24, 67.5164, 56781.2, 7.1d+5 Length(cm), Diam(cm), Q-flow(ml/min), CSTR-vol(ml)
172.0, 0.50, 0.240, 0.0
                                  part-rad(um), bed-void, part-void, sorb-cap()
                                  initial concentrations (M)
 0.0
                                  COMMAND - conc step change
1, 0.0, 2.4546d-5, 1, 0.0
                                  spec id, time(min), conc(M), freq, dt(min)
                                  COMMAND - viscosity/density change
                                  fluid viscosity(posie), density(g/cm^3)
0.026463, 1.2964
                                  COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5
                                  unit op#, ptscale(1-4) filtering
D
-1, 6012.64, 1, 0.0
-1, 13947.8, 1, 0.0
                                  end of commands
66667.0, 1.0
                                  end time(min), max dt in B.V.s
1.0d-7, 1.0d-4
                                  abs-tol, rel-tol
                                  non-negative conc constraint
1.0d0
                                  size exclusion factor
                                  part-pore diffusivities(cm^2/min) 20% of free value
7.569d-5
3.785d-4
                                  Brownian diffusivities(cm<sup>2</sup>/min)
0.3943
                                  Freundlich/Langmuir Hybrid a
                                                                   (moles/L B.V.) rhob=1.0 g/ml
1.0
                                  Freundlich/Langmuir Hybrid b
                                                                   (1/M) Batch specific isotherm
1.0
                                  Freundlich/Langmuir Hybrid Ma
                                                                   (-)
1.0
                                  Freundlich/Langmuir Hybrid Mb
                                                                   (-)
                                  Freundlich/Langmuir Hybrid beta (-)
```

## VERSE Input: Design 6 with Batch 6 feed stream

```
Design 6, IE-911, L=13ft,D=26.6in,V=375Gal,F=15gpm,T=30C
1 component (Cs) isotherm (Batch 6)
1, 50, 3, 6
                                 ncomp, nelem, ncol-bed, ncol-part
FCWNA
                                  isotherm,axial-disp,film-coef,surf-diff,BC-col FCUNA
NNNNN
                                 input-only, perfusable, feed-equil, datafile. yio
                                 comp-conc units
396.24, 67.5164, 56781.2, 7.1d+5 Length(cm), Diam(cm), Q-flow(ml/min), CSTR-vol(ml)
172.0, 0.50, 0.240, 0.0
                                 part-rad(um), bed-void, part-void, sorb-cap()
  0.0
                                 initial concentrations (M)
                                 COMMAND - conc step change
1, 0.0, 7.7688d-5, 1, 0.0
                                 spec id, time(min), conc(M), freq, dt(min)
                                 COMMAND - viscosity/density change
0.026399, 1.2626
                                 fluid viscosity(posie), density(g/cm^3)
                                 COMMAND - effluent history dump
2, 1.0, 1.0, 0.50, 0.5
                                 unit op#, ptscale(1-4) filtering
-1, 7944.62, 1, 0.0
-1, 14609.3, 1, 0.0
                                 end of commands
66667.0, 1.0
                                 end time(min), max dt in B.V.s
1.0d-7, 1.0d-4
                                 abs-tol, rel-tol
                                 non-negative conc constraint
1.0d0
                                 size exclusion factor
8.235d-5
                                 part-pore diffusivities(cm^2/min) 20% of free value
4.117d-4
                                 Brownian diffusivities(cm^2/min)
0.3943
                                 Freundlich/Langmuir Hybrid a
                                                                (moles/L B.V.) rhob=1.0 g/ml
```

```
1.0 Freundlich/Langmuir Hybrid b (1/M) Batch specific isotherm
1.0 Freundlich/Langmuir Hybrid Ma (-)
1.0 Freundlich/Langmuir Hybrid Mb (-)
4.9272d-4 Freundlich/Langmuir Hybrid beta (-)
```

## VERSE Input: Design 6 with Batch 8 feed stream

```
Design 6, IE-911, L=13ft,D=26.6in,V=375Gal,F=15gpm,T=30C
1 component (Cs) isotherm (Batch 8)
1, 50, 3, 6
                                  ncomp, nelem, ncol-bed, ncol-part
FCWNA
                                  isotherm, axial-disp, film-coef, surf-diff, BC-col FCUNA
NNNNN
                                  input-only,perfusable,feed-equil,datafile.yio
                                  comp-conc units
396.24, 67.5164, 56781.2, 7.1d+5 Length(cm), Diam(cm), Q-flow(ml/min), CSTR-vol(ml)
172.0, 0.50, 0.240, 0.0
                                  part-rad(um), bed-void, part-void, sorb-cap()
  0.0
                                  initial concentrations (M)
                                  COMMAND - conc step change
1, 0.0, 3.9625d-5, 1, 0.0
                                  spec id, time(min), conc(M), freq, dt(min)
                                  COMMAND - viscosity/density change
0.030909, 1.2372
                                  fluid viscosity(posie), density(g/cm^3)
                                  COMMAND - effluent history dump
h
2, 1.0, 1.0, 0.50, 0.5
                                  unit op#, ptscale(1-4) filtering
D
-1, 10676.00, 1, 0.0
-1, 21389.10, 1, 0.0
                                  end of commands
66667.0, 1.0
                                  end time(min), max dt in B.V.s
1.0d-7, 1.0d-4
                                  abs-tol, rel-tol
                                  non-negative conc constraint
1.0d0
                                  size exclusion factor
7.953d-5
                                  part-pore diffusivities(cm^2/min) 20% of free value
3.976d-4
                                  Brownian diffusivities(cm^2/min)
0.3938
                                  Freundlich/Langmuir Hybrid a
                                                                   (moles/L B.V.) rhob=1.0 g/ml
1.0
                                  Freundlich/Langmuir Hybrid b
                                                                   (1/M) Batch specific isotherm
1.0
                                  Freundlich/Langmuir Hybrid Ma
                                                                   (-)
                                  Freundlich/Langmuir Hybrid Mb
1.0
                                                                   (-)
3.9421d-4
                                  Freundlich/Langmuir Hybrid beta (-)
```

# Appendix B

## MAR Results for Nominal Stage Assessments For the "Original" SB4 Composition

Table B.1. MAR Assessment and Various Predicted Properties.

| Category              | WL  | B \( \Delta G p \) | B \( \Delta \G p \) | T <sub>L</sub> Pred | $T_{ m L}$ | Visc    | TiO <sub>2</sub> | Sum of | MAR              |
|-----------------------|-----|--------------------|---------------------|---------------------|------------|---------|------------------|--------|------------------|
|                       | (%) | MAR                | Value               | (°C)                | MAR(°C)    | Pred    | wt%              | Alkali | Status           |
|                       |     |                    |                     |                     |            | (Poise) |                  | wt%    |                  |
| 320-Original Baseline | 25  | -13.7200           | -10.7378            | 891.51              | 996.60     | 65.57   | 0.000            | 18.28  | -                |
| 320-Original Baseline | 26  | -13.7200           | -10.6449            | 913.14              | 997.78     | 64.51   | 0.000            | 18.22  | -                |
| 320-Original Baseline | 27  | -13.7200           | -10.5519            | 934.43              | 998.70     | 63.44   | 0.000            | 18.15  | -                |
| 320-Original Baseline | 28  | -13.7200           | -10.4590            | 955.37              | 999.29     | 62.36   | 0.000            | 18.08  | -                |
| 320-Original Baseline | 29  | -13.7200           | -10.3661            | 975.98              | 999.50     | 61.27   | 0.000            | 18.01  | -                |
| 320-Original Baseline | 30  | -13.7200           | -10.2731            | 996.27              | 999.29     | 60.17   | 0.000            | 17.94  | -                |
| 320-Original Baseline | 31  | -13.7200           | -10.1802            | 1016.26             | 998.69     | 59.06   | 0.000            | 17.87  | $T_{ m L}$       |
| 320-Original Baseline | 32  | -13.7200           | -10.0872            | 1035.94             | 997.75     | 57.95   | 0.000            | 17.80  | $T_{ m L}$       |
| 320-Original Baseline | 33  | -13.7200           | -9.9943             | 1055.34             | 996.52     | 56.82   | 0.000            | 17.74  | $T_{ m L}$       |
| 320-Original Baseline | 34  | -13.7200           | -9.9014             | 1074.45             | 995.06     | 55.69   | 0.000            | 17.67  | $T_{ m L}$       |
| 320-Original Baseline | 35  | -13.7200           | -9.8084             | 1093.28             | 993.42     | 54.54   | 0.000            | 17.60  | $T_{ m L}$       |
| 320-Original Baseline | 36  | -13.7200           | -9.7155             | 1111.85             | 991.63     | 53.39   | 0.000            | 17.53  | $T_{ m L}$       |
| 320-Original Baseline | 37  | -13.7200           | -9.6226             | 1130.15             | 989.73     | 52.23   | 0.000            | 17.46  | $T_{ m L}$       |
| 320-Original Baseline | 38  | -13.7200           | -9.5296             | 1148.19             | 987.73     | 51.07   | 0.000            | 17.39  | $T_{ m L}$       |
| 320-Original Baseline | 39  | -13.7200           | -9.4367             | 1165.98             | 985.66     | 49.89   | 0.000            | 17.32  | $T_{ m L}$       |
| 320-Original Baseline | 40  | -13.7200           | -9.3437             | 1183.53             | 983.52     | 48.71   | 0.000            | 17.26  | $T_{ m L}$       |
| 320-Original Baseline | 41  | -13.7200           | -9.2508             | 1200.84             | 981.32     | 47.52   | 0.000            | 17.19  | $T_{ m L}$       |
| 320-Original Baseline | 42  | -13.7200           | -9.1579             | 1217.91             | 979.07     | 46.32   | 0.000            | 17.12  | $T_{ m L}$       |
| 320-Original Baseline | 43  | -13.7200           | -9.0649             | 1234.75             | 976.77     | 45.12   | 0.000            | 17.05  | $T_{ m L}$       |
| 320-Original Baseline | 44  | -13.7200           | -8.9720             | 1251.36             | 974.44     | 43.91   | 0.000            | 16.98  | $T_{ m L}$       |
| 320-Original Baseline | 45  | -13.7200           | -8.8790             | 1267.75             | 972.07     | 42.69   | 0.000            | 16.91  | $T_{ m L}$       |
| 320-Original Baseline | 46  | -13.7200           | -8.7861             | 1283.93             | 969.67     | 41.47   | 0.000            | 16.84  | $T_{\mathrm{L}}$ |
| 320-Original Baseline | 47  | -13.7200           | -8.6932             | 1299.89             | 967.24     | 40.24   | 0.000            | 16.77  | $T_{\mathrm{L}}$ |
| 320-Original Baseline | 48  | -13.7200           | -8.6002             | 1315.65             | 964.79     | 39.01   | 0.000            | 16.71  | $T_{ m L}$       |
| 320-Original Baseline | 49  | -13.7200           | -8.5073             | 1331.20             | 962.31     | 37.78   | 0.000            | 16.64  | $T_{ m L}$       |
| 320-Original Baseline | 50  | -13.7200           | -8.4143             | 1346.54             | 959.81     | 36.54   | 0.000            | 16.57  | $T_{\mathrm{L}}$ |

| Category                    | WL<br>(%) | B ΔGp<br>MAR | B ∆Gp<br>Value | T <sub>L</sub> Pred<br>(°C) | T <sub>L</sub><br>MAR(°C) | Visc<br>Pred<br>(Poise) | TiO <sub>2</sub> wt% | Sum of<br>Alkali<br>wt% | MAR<br>Status          |
|-----------------------------|-----------|--------------|----------------|-----------------------------|---------------------------|-------------------------|----------------------|-------------------------|------------------------|
| 320-Original Baseline       | 51        | -13.7200     | -8.3214        | 1361.70                     | 957.30                    | 35.30                   | 0.000                | 16.50                   | $T_{ m L}$             |
| 320-Original Baseline       | 52        | -13.7200     | -8.2285        | 1376.65                     | 954.76                    | 34.05                   | 0.000                | 16.43                   | $T_{\rm L}$            |
| 320-Original Baseline       | 53        | -13.7200     | -8.1355        | 1391.42                     | 952.21                    | 32.81                   | 0.000                | 16.36                   | $T_{\rm L}$            |
| 320-Original Baseline       | 54        | -13.7200     | -8.0426        | 1406.00                     | 949.64                    | 31.57                   | 0.000                | 16.29                   | $T_{\rm L}$            |
| 320-Original Baseline       | 55        | -13.7200     | -7.9496        | 1420.39                     | 947.06                    | 30.32                   | 0.000                | 16.23                   | $T_{\rm L}$            |
| 320-Original Baseline       | 56        | -13.7200     | -7.8567        | 1434.60                     | 944.47                    | 29.08                   | 0.000                | 16.16                   | $T_{\rm L}$            |
| 320-Original Baseline       | 57        | -13.7200     | -7.7638        | 1448.64                     | 941.87                    | 27.84                   | 0.000                | 16.09                   | $T_{\rm L}$            |
| 320-Original Baseline       | 58        | -13.7200     | -7.6708        | 1462.50                     | 939.25                    | 26.60                   | 0.000                | 16.02                   | $T_{ m L}$             |
| 320-Original Baseline       | 59        | -13.7200     | -7.5779        | 1476.19                     | 936.63                    | 25.37                   | 0.000                | 15.95                   | T <sub>L</sub> , low η |
| 320-Original Baseline       | 60        | -13.7200     | -7.4850        | 1489.71                     | 934.00                    | 24.15                   | 0.000                | 15.88                   | $T_L$ , low $\eta$     |
| 320-Original Baseline w CST | 25        | -13.7200     | -10.7281       | 856.57                      | 995.85                    | 66.26                   | 0.770                | 18.34                   | -                      |
| 320-Original Baseline w CST | 26        | -13.7200     | -10.6347       | 877.00                      | 997.28                    | 65.23                   | 0.801                | 18.27                   | -                      |
| 320-Original Baseline w CST | 27        | -13.7200     | -10.5414       | 897.09                      | 998.61                    | 64.19                   | 0.832                | 18.20                   | -                      |
| 320-Original Baseline w CST | 28        | -13.7200     | -10.4481       | 916.84                      | 999.81                    | 63.14                   | 0.863                | 18.14                   | -                      |
| 320-Original Baseline w CST | 29        | -13.7200     | -10.3547       | 936.27                      | 1000.81                   | 62.09                   | 0.893                | 18.07                   | -                      |
| 320-Original Baseline w CST | 30        | -13.7200     | -10.2614       | 955.39                      | 1001.57                   | 61.02                   | 0.924                | 18.00                   | -                      |
| 320-Original Baseline w CST | 31        | -13.7200     | -10.1681       | 974.20                      | 1002.01                   | 59.95                   | 0.955                | 17.94                   | -                      |
| 320-Original Baseline w CST | 32        | -13.7200     | -10.0748       | 992.71                      | 1002.12                   | 58.87                   | 0.986                | 17.87                   | -                      |
| 320-Original Baseline w CST | 33        | -13.7200     | -9.9814        | 1010.94                     | 1001.87                   | 57.77                   | 1.017                | 17.80                   | $T_{ m L}$             |
| 320-Original Baseline w CST | 34        | -13.7200     | -9.8881        | 1028.89                     | 1001.28                   | 56.67                   | 1.048                | 17.74                   | $T_{ m L}$             |
| 320-Original Baseline w CST | 35        | -13.7200     | -9.7948        | 1046.56                     | 1000.41                   | 55.57                   | 1.078                | 17.67                   | $T_{ m L}$             |
| 320-Original Baseline w CST | 36        | -13.7200     | -9.7014        | 1063.97                     | 999.30                    | 54.45                   | 1.109                | 17.60                   | $T_{ m L}$             |
| 320-Original Baseline w CST | 37        | -13.7200     | -9.6081        | 1081.13                     | 998.01                    | 53.32                   | 1.140                | 17.54                   | $T_{ m L}$             |
| 320-Original Baseline w CST | 38        | -13.7200     | -9.5148        | 1098.02                     | 996.56                    | 52.19                   | 1.171                | 17.47                   | $T_{ m L}$             |
| 320-Original Baseline w CST | 39        | -13.7200     | -9.4215        | 1114.68                     | 995.00                    | 51.05                   | 1.202                | 17.40                   | $T_{ m L}$             |
| 320-Original Baseline w CST | 40        | -13.7200     | -9.3281        | 1131.09                     | 993.35                    | 49.90                   | 1.232                | 17.34                   | $T_{ m L}$             |
| 320-Original Baseline w CST | 41        | -13.7200     | -9.2348        | 1147.26                     | 991.61                    | 48.75                   | 1.263                | 17.27                   | $T_{\rm L}$            |
| 320-Original Baseline w CST | 42        | -13.7200     | -9.1415        | 1163.20                     | 989.81                    | 47.58                   | 1.294                | 17.20                   | $T_{\rm L}$            |

| Category                    | WL  | B ∆Gp    | B ∆Gp   | T <sub>L</sub> Pred | $T_{ m L}$ | Visc    | TiO <sub>2</sub> | Sum of | MAR         |
|-----------------------------|-----|----------|---------|---------------------|------------|---------|------------------|--------|-------------|
|                             | (%) | MAR      | Value   | (°C)                | MAR(°C)    | Pred    | wt%              | Alkali | Status      |
|                             |     |          |         |                     |            | (Poise) |                  | wt%    |             |
| 320-Original Baseline w CST | 43  | -13.7200 | -9.0481 | 1178.92             | 987.96     | 46.41   | 1.325            | 17.14  | $T_{ m L}$  |
| 320-Original Baseline w CST | 44  | -13.7200 | -8.9548 | 1194.42             | 986.07     | 45.24   | 1.356            | 17.07  | $T_{ m L}$  |
| 320-Original Baseline w CST | 45  | -13.7200 | -8.8615 | 1209.69             | 984.13     | 44.06   | 1.386            | 17.00  | ${ m T_L}$  |
| 320-Original Baseline w CST | 46  | -13.7200 | -8.7681 | 1224.76             | 982.16     | 42.87   | 1.417            | 16.94  | $T_{ m L}$  |
| 320-Original Baseline w CST | 47  | -13.7200 | -8.6748 | 1239.61             | 980.16     | 41.67   | 1.448            | 16.87  | $T_{ m L}$  |
| 320-Original Baseline w CST | 48  | -13.7200 | -8.5815 | 1254.26             | 978.14     | 40.47   | 1.479            | 16.80  | $T_{ m L}$  |
| 320-Original Baseline w CST | 49  | -13.7200 | -8.4882 | 1268.72             | 976.09     | 39.27   | 1.510            | 16.74  | $T_{ m L}$  |
| 320-Original Baseline w CST | 50  | -13.7200 | -8.3948 | 1282.97             | 974.03     | 38.06   | 1.541            | 16.67  | $T_{\rm L}$ |
| 320-Original Baseline w CST | 51  | -13.7200 | -8.3015 | 1297.03             | 971.94     | 36.85   | 1.571            | 16.60  | $T_{ m L}$  |
| 320-Original Baseline w CST | 52  | -13.7200 | -8.2082 | 1310.90             | 969.84     | 35.64   | 1.602            | 16.54  | $T_{\rm L}$ |
| 320-Original Baseline w CST | 53  | -13.7200 | -8.1148 | 1324.58             | 967.72     | 34.42   | 1.633            | 16.47  | $T_{\rm L}$ |
| 320-Original Baseline w CST | 54  | -13.7200 | -8.0215 | 1338.08             | 965.59     | 33.20   | 1.664            | 16.40  | $T_{ m L}$  |
| 320-Original Baseline w CST | 55  | -13.7200 | -7.9282 | 1351.40             | 963.45     | 31.98   | 1.695            | 16.34  | $T_{ m L}$  |
| 320-Original Baseline w CST | 56  | -13.7200 | -7.8349 | 1364.54             | 961.30     | 30.77   | 1.725            | 16.27  | $T_{ m L}$  |
| 320-Original Baseline w CST | 57  | -13.7200 | -7.7415 | 1377.51             | 959.14     | 29.55   | 1.756            | 16.20  | $T_{\rm L}$ |
| 320-Original Baseline w CST | 58  | -13.7200 | -7.6482 | 1390.31             | 956.98     | 28.33   | 1.787            | 16.14  | $T_{ m L}$  |
| 320-Original Baseline w CST | 59  | -13.7200 | -7.5549 | 1402.94             | 954.81     | 27.12   | 1.818            | 16.07  | $T_{ m L}$  |
| 320-Original Baseline w CST | 60  | -13.7200 | -7.4615 | 1415.41             | 952.63     | 25.91   | 1.849            | 16.00  | $T_{\rm L}$ |

# **Appendix C**

MAR Results for Nominal Stage Assessments
For the Alternative Frits and the Revised SB4 Compositions and Masses

Table C.1 MAR Based Assessments and Various Predicted Properties for the Revised SB4 Compositions and Masses.

| Category              | WL  | B \( \Delta \G p \) | B \( \Delta \G p \) | $T_{ m L}$ | $T_{ m L}$ | Visc       | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                 |
|-----------------------|-----|---------------------|---------------------|------------|------------|------------|------------------|------------------|---------------------|
| January J             | (%) | MAR                 | Value               | Pred       | MAR(°C)    | Pred       | wt%              | wt%              | Status              |
|                       |     |                     |                     | (°C)       | ,          | <b>(P)</b> |                  |                  |                     |
| 418-Original Baseline | 25  | -13.7200            | -7.9659             | 956.16     | 999.14     | 111.29     | 0.000            | 15.28            | high η              |
| 418-Original Baseline | 26  | -13.7200            | -7.9099             | 978.15     | 999.24     | 109.53     | 0.000            | 15.26            | high η              |
| 418-Original Baseline | 27  | -13.7200            | -7.8539             | 999.71     | 998.88     | 107.75     | 0.000            | 15.23            | $T_L$ , high $\eta$ |
| 418-Original Baseline | 28  | -13.7200            | -7.7979             | 1020.85    | 998.11     | 105.96     | 0.000            | 15.20            | $T_L$ , high $\eta$ |
| 418-Original Baseline | 29  | -13.7200            | -7.7419             | 1041.59    | 997.00     | 104.15     | 0.000            | 15.17            | $T_L$ , high $\eta$ |
| 418-Original Baseline | 30  | -13.7200            | -7.6860             | 1061.94    | 995.60     | 102.33     | 0.000            | 15.14            | $T_L$ , high $\eta$ |
| 418-Original Baseline | 31  | -13.7200            | -7.6300             | 1081.92    | 993.98     | 100.49     | 0.000            | 15.11            | $T_L$ , high $\eta$ |
| 418-Original Baseline | 32  | -13.7200            | -7.5740             | 1101.54    | 992.19     | 98.63      | 0.000            | 15.08            | $T_{\rm L}$         |
| 418-Original Baseline | 33  | -13.7200            | -7.5180             | 1120.80    | 990.27     | 96.76      | 0.000            | 15.06            | $T_{L}$             |
| 418-Original Baseline | 34  | -13.7200            | -7.4620             | 1139.72    | 988.25     | 94.87      | 0.000            | 15.03            | $T_{ m L}$          |
| 418-Original Baseline | 35  | -13.7200            | -7.4061             | 1158.31    | 986.13     | 92.97      | 0.000            | 15.00            | $T_{ m L}$          |
| 418-Original Baseline | 36  | -13.7200            | -7.3501             | 1176.58    | 983.95     | 91.05      | 0.000            | 14.97            | $T_{ m L}$          |
| 418-Original Baseline | 37  | -13.7200            | -7.2941             | 1194.53    | 981.71     | 89.12      | 0.000            | 14.94            | $T_{ m L}$          |
| 418-Original Baseline | 38  | -13.7200            | -7.2381             | 1212.18    | 979.42     | 87.17      | 0.000            | 14.91            | $T_{ m L}$          |
| 418-Original Baseline | 39  | -13.7200            | -7.1821             | 1229.53    | 977.09     | 85.21      | 0.000            | 14.88            | $T_{ m L}$          |
| 418-Original Baseline | 40  | -13.7200            | -7.1262             | 1246.59    | 974.72     | 83.23      | 0.000            | 14.86            | $T_{ m L}$          |
| 418-Original Baseline | 41  | -13.7200            | -7.0702             | 1263.36    | 972.32     | 81.24      | 0.000            | 14.83            | $T_{ m L}$          |
| 418-Original Baseline | 42  | -13.7200            | -7.0142             | 1279.86    | 969.90     | 79.24      | 0.000            | 14.80            | $T_{ m L}$          |
| 418-Original Baseline | 43  | -13.7200            | -6.9582             | 1296.09    | 967.45     | 77.23      | 0.000            | 14.77            | $T_{ m L}$          |
| 418-Original Baseline | 44  | -13.7200            | -6.9023             | 1312.06    | 964.98     | 75.20      | 0.000            | 14.74            | $T_{ m L}$          |
| 418-Original Baseline | 45  | -13.7200            | -6.8463             | 1327.77    | 962.50     | 73.16      | 0.000            | 14.71            | $T_{ m L}$          |
| 418-Original Baseline | 46  | -13.7200            | -6.7903             | 1343.23    | 960.00     | 71.11      | 0.000            | 14.68            | $T_{ m L}$          |
| 418-Original Baseline | 47  | -13.7200            | -6.7343             | 1358.45    | 957.49     | 69.05      | 0.000            | 14.65            | $T_{ m L}$          |
| 418-Original Baseline | 48  | -13.7200            | -6.6783             | 1373.43    | 954.97     | 66.98      | 0.000            | 14.63            | $T_{ m L}$          |
| 418-Original Baseline | 49  | -13.7200            | -6.6224             | 1388.17    | 952.44     | 64.90      | 0.000            | 14.60            | $T_{ m L}$          |
| 418-Original Baseline | 50  | -13.7200            | -6.5664             | 1402.68    | 949.90     | 62.82      | 0.000            | 14.57            | $T_{ m L}$          |
| 418-Original Baseline | 51  | -13.7200            | -6.5104             | 1416.97    | 947.35     | 60.73      | 0.000            | 14.54            | $T_{ m L}$          |

| Category                    | WL  | B ∆Gp    | B ∆Gp   | $T_{\rm L}$ | $T_{\rm L}$ | Visc   | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                     |
|-----------------------------|-----|----------|---------|-------------|-------------|--------|------------------|------------------|-------------------------|
|                             | (%) | MAR      | Value   | Pred        | MAR(°C)     | Pred   | wt%              | wt%              | Status                  |
|                             |     |          |         | (°C)        |             | (P)    |                  |                  |                         |
| 418-Original Baseline       | 52  | -13.7200 | -6.4544 | 1431.05     | 944.80      | 58.63  | 0.000            | 14.51            | $T_{ m L}$              |
| 418-Original Baseline       | 53  | -13.7200 | -6.3984 | 1444.90     | 942.25      | 56.53  | 0.000            | 14.48            | $T_{ m L}$              |
| 418-Original Baseline       | 54  | -13.7200 | -6.3425 | 1458.55     | 939.70      | 54.43  | 0.000            | 14.45            | $T_{ m L}$              |
| 418-Original Baseline       | 55  | -13.7200 | -6.2865 | 1472.00     | 937.14      | 52.32  | 0.000            | 14.43            | $T_{ m L}$              |
| 418-Original Baseline       | 56  | -13.7200 | -6.2305 | 1485.24     | 934.58      | 50.22  | 0.000            | 14.40            | $T_{ m L}$              |
| 418-Original Baseline       | 57  | -13.7200 | -6.1745 | 1498.29     | 932.03      | 48.12  | 0.000            | 14.37            | $T_{\rm L}$             |
| 418-Original Baseline       | 58  | -13.7200 | -6.1185 | 1511.14     | 929.47      | 46.02  | 0.000            | 14.34            | $T_{ m L}$              |
| 418-Original Baseline       | 59  | -13.7200 | -6.0626 | 1523.81     | 926.92      | 43.93  | 0.000            | 14.31            | $T_{ m L}$              |
| 418-Original Baseline       | 60  | -13.7200 | -6.0066 | 1536.29     | 924.37      | 41.85  | 0.000            | 14.28            | $T_{ m L}$              |
| 418-Original Baseline w CST | 25  | -13.7200 | -7.9561 | 918.31      | 999.97      | 112.04 | 0.770            | 15.34            | high η                  |
| 418-Original Baseline w CST | 26  | -13.7200 | -7.8997 | 939.04      | 1000.93     | 110.32 | 0.801            | 15.31            | high η                  |
| 418-Original Baseline w CST | 27  | -13.7200 | -7.8434 | 959.34      | 1001.58     | 108.58 | 0.832            | 15.28            | high η                  |
| 418-Original Baseline w CST | 28  | -13.7200 | -7.7870 | 979.24      | 1001.88     | 106.83 | 0.863            | 15.26            | high η                  |
| 418-Original Baseline w CST | 29  | -13.7200 | -7.7306 | 998.74      | 1001.79     | 105.06 | 0.893            | 15.23            | high η                  |
| 418-Original Baseline w CST | 30  | -13.7200 | -7.6743 | 1017.87     | 1001.33     | 103.27 | 0.924            | 15.20            | T <sub>L</sub> , high η |
| 418-Original Baseline w CST | 31  | -13.7200 | -7.6179 | 1036.62     | 1000.54     | 101.48 | 0.955            | 15.18            | $T_L$ , high $\eta$     |
| 418-Original Baseline w CST | 32  | -13.7200 | -7.5615 | 1055.03     | 999.48      | 99.66  | 0.986            | 15.15            | $T_{ m L}$              |
| 418-Original Baseline w CST | 33  | -13.7200 | -7.5051 | 1073.08     | 998.20      | 97.83  | 1.017            | 15.12            | $T_{ m L}$              |
| 418-Original Baseline w CST | 34  | -13.7200 | -7.4488 | 1090.81     | 996.76      | 95.99  | 1.048            | 15.10            | $T_{ m L}$              |
| 418-Original Baseline w CST | 35  | -13.7200 | -7.3924 | 1108.21     | 995.18      | 94.13  | 1.078            | 15.07            | $T_{\rm L}$             |
| 418-Original Baseline w CST | 36  | -13.7200 | -7.3360 | 1125.29     | 993.50      | 92.26  | 1.109            | 15.04            | $T_{\rm L}$             |
| 418-Original Baseline w CST | 37  | -13.7200 | -7.2797 | 1142.07     | 991.74      | 90.37  | 1.140            | 15.02            | $T_{L}$                 |
| 418-Original Baseline w CST | 38  | -13.7200 | -7.2233 | 1158.55     | 989.92      | 88.47  | 1.171            | 14.99            | $T_{\rm L}$             |
| 418-Original Baseline w CST | 39  | -13.7200 | -7.1669 | 1174.73     | 988.04      | 86.55  | 1.202            | 14.96            | $T_{L}$                 |
| 418-Original Baseline w CST | 40  | -13.7200 | -7.1106 | 1190.64     | 986.12      | 84.62  | 1.232            | 14.94            | $T_{\rm L}$             |
| 418-Original Baseline w CST | 41  | -13.7200 | -7.0542 | 1206.27     | 984.16      | 82.68  | 1.263            | 14.91            | $T_{\rm L}$             |
| 418-Original Baseline w CST | 42  | -13.7200 | -6.9978 | 1221.63     | 982.17      | 80.73  | 1.294            | 14.88            | $T_{ m L}$              |
| 418-Original Baseline w CST | 43  | -13.7200 | -6.9414 | 1236.73     | 980.16      | 78.76  | 1.325            | 14.86            | $T_{ m L}$              |
| 418-Original Baseline w CST | 44  | -13.7200 | -6.8851 | 1251.58     | 978.13      | 76.78  | 1.356            | 14.83            | $T_{\rm L}$             |
| 418-Original Baseline w CST | 45  | -13.7200 | -6.8287 | 1266.17     | 976.08      | 74.79  | 1.386            | 14.80            | $T_{\rm L}$             |
| 418-Original Baseline w CST | 46  | -13.7200 | -6.7723 | 1280.52     | 974.01      | 72.79  | 1.417            | 14.78            | $T_{\rm L}$             |

| Category                    | WL  | B ∆Gp    | B ∆Gp    | $T_{ m L}$ | $T_{ m L}$ | Visc       | TiO <sub>2</sub> | R <sub>2</sub> O | MAR        |
|-----------------------------|-----|----------|----------|------------|------------|------------|------------------|------------------|------------|
|                             | (%) | MAR      | Value    | Pred       | MAR(°C)    | Pred       | wt%              | wt%              | Status     |
|                             |     |          |          | (°C)       |            | <b>(P)</b> |                  |                  |            |
| 418-Original Baseline w CST | 47  | -13.7200 | -6.7160  | 1294.63    | 971.93     | 70.77      | 1.448            | 14.75            | $T_{ m L}$ |
| 418-Original Baseline w CST | 48  | -13.7200 | -6.6596  | 1308.51    | 969.84     | 68.75      | 1.479            | 14.72            | $T_{ m L}$ |
| 418-Original Baseline w CST | 49  | -13.7200 | -6.6032  | 1322.17    | 967.74     | 66.72      | 1.510            | 14.70            | $T_{ m L}$ |
| 418-Original Baseline w CST | 50  | -13.7200 | -6.5469  | 1335.60    | 965.64     | 64.68      | 1.541            | 14.67            | $T_{ m L}$ |
| 418-Original Baseline w CST | 51  | -13.7200 | -6.4905  | 1348.82    | 963.53     | 62.64      | 1.571            | 14.64            | $T_{ m L}$ |
| 418-Original Baseline w CST | 52  | -13.7200 | -6.4341  | 1361.82    | 961.42     | 60.59      | 1.602            | 14.62            | $T_{ m L}$ |
| 418-Original Baseline w CST | 53  | -13.7200 | -6.3777  | 1374.62    | 959.30     | 58.53      | 1.633            | 14.59            | $T_{ m L}$ |
| 418-Original Baseline w CST | 54  | -13.7200 | -6.3214  | 1387.21    | 957.19     | 56.47      | 1.664            | 14.56            | $T_{ m L}$ |
| 418-Original Baseline w CST | 55  | -13.7200 | -6.2650  | 1399.61    | 955.07     | 54.41      | 1.695            | 14.54            | $T_{ m L}$ |
| 418-Original Baseline w CST | 56  | -13.7200 | -6.2086  | 1411.81    | 952.95     | 52.35      | 1.725            | 14.51            | $T_{ m L}$ |
| 418-Original Baseline w CST | 57  | -13.7200 | -6.1523  | 1423.82    | 950.84     | 50.29      | 1.756            | 14.48            | $T_{ m L}$ |
| 418-Original Baseline w CST | 58  | -13.7200 | -6.0959  | 1435.65    | 948.72     | 48.23      | 1.787            | 14.46            | $T_{ m L}$ |
| 418-Original Baseline w CST | 59  | -13.7200 | -6.0395  | 1447.29    | 946.61     | 46.18      | 1.818            | 14.43            | $T_{ m L}$ |
| 418-Original Baseline w CST | 60  | -13.7200 | -5.9832  | 1458.76    | 944.51     | 44.13      | 1.849            | 14.40            | $T_{ m L}$ |
| 440-Original Baseline       | 25  | -13.6604 | -12.9628 | 848.95     | 991.97     | 73.52      | 0.000            | 20.53            | -          |
| 440-Original Baseline       | 26  | -13.6644 | -12.8402 | 869.98     | 993.52     | 72.28      | 0.000            | 20.44            | -          |
| 440-Original Baseline       | 27  | -13.6683 | -12.7175 | 890.71     | 994.98     | 71.02      | 0.000            | 20.34            | -          |
| 440-Original Baseline       | 28  | -13.6723 | -12.5949 | 911.14     | 996.34     | 69.76      | 0.000            | 20.24            | -          |
| 440-Original Baseline       | 29  | -13.6763 | -12.4723 | 931.29     | 997.52     | 68.49      | 0.000            | 20.14            | -          |
| 440-Original Baseline       | 30  | -13.6803 | -12.3497 | 951.17     | 998.48     | 67.21      | 0.000            | 20.04            | -          |
| 440-Original Baseline       | 31  | -13.6842 | -12.2271 | 970.79     | 999.14     | 65.91      | 0.000            | 19.94            | -          |
| 440-Original Baseline       | 32  | -13.6882 | -12.1045 | 990.14     | 999.46     | 64.61      | 0.000            | 19.84            | -          |
| 440-Original Baseline       | 33  | -13.6921 | -11.9819 | 1009.25    | 999.38     | 63.30      | 0.000            | 19.75            | $T_{ m L}$ |
| 440-Original Baseline       | 34  | -13.6961 | -11.8593 | 1028.12    | 998.92     | 61.99      | 0.000            | 19.65            | $T_{ m L}$ |
| 440-Original Baseline       | 35  | -13.7000 | -11.7367 | 1046.75    | 998.11     | 60.66      | 0.000            | 19.55            | $T_{ m L}$ |
| 440-Original Baseline       | 36  | -13.7039 | -11.6141 | 1065.16    | 997.01     | 59.32      | 0.000            | 19.45            | $T_{ m L}$ |
| 440-Original Baseline       | 37  | -13.7078 | -11.4915 | 1083.34    | 995.67     | 57.98      | 0.000            | 19.35            | $T_{ m L}$ |
| 440-Original Baseline       | 38  | -13.7117 | -11.3689 | 1101.30    | 994.14     | 56.63      | 0.000            | 19.25            | $T_{ m L}$ |
| 440-Original Baseline       | 39  | -13.7156 | -11.2463 | 1119.05    | 992.46     | 55.27      | 0.000            | 19.15            | $T_{ m L}$ |
| 440-Original Baseline       | 40  | -13.7195 | -11.1237 | 1136.60    | 990.66     | 53.90      | 0.000            | 19.06            | $T_{ m L}$ |
| 440-Original Baseline       | 41  | -13.7200 | -11.0011 | 1153.94    | 988.75     | 52.53      | 0.000            | 18.96            | $T_{ m L}$ |
| 440-Original Baseline       | 42  | -13.7200 | -10.8785 | 1171.08    | 986.75     | 51.15      | 0.000            | 18.86            | $T_{ m L}$ |

| Category                    | WL  | B ∆Gp    | B ∆Gp    | $T_{\rm L}$ | $T_{\rm L}$ | Visc  | TiO <sub>2</sub> | R <sub>2</sub> O | MAR        |
|-----------------------------|-----|----------|----------|-------------|-------------|-------|------------------|------------------|------------|
|                             | (%) | MAR      | Value    | Pred        | MAR(°C)     | Pred  | wt%              | wt%              | Status     |
|                             |     |          |          | (°C)        |             | (P)   |                  |                  |            |
| 440-Original Baseline       | 43  | -13.7200 | -10.7559 | 1188.03     | 984.69      | 49.76 | 0.000            | 18.76            | $T_{ m L}$ |
| 440-Original Baseline       | 44  | -13.7200 | -10.6333 | 1204.79     | 982.56      | 48.37 | 0.000            | 18.66            | $T_{ m L}$ |
| 440-Original Baseline       | 45  | -13.7200 | -10.5107 | 1221.36     | 980.37      | 46.97 | 0.000            | 18.56            | $T_{ m L}$ |
| 440-Original Baseline       | 46  | -13.7200 | -10.3881 | 1237.75     | 978.13      | 45.57 | 0.000            | 18.46            | $T_{ m L}$ |
| 440-Original Baseline       | 47  | -13.7200 | -10.2654 | 1253.95     | 975.85      | 44.17 | 0.000            | 18.36            | $T_{ m L}$ |
| 440-Original Baseline       | 48  | -13.7200 | -10.1428 | 1269.99     | 973.52      | 42.76 | 0.000            | 18.27            | $T_{ m L}$ |
| 440-Original Baseline       | 49  | -13.7200 | -10.0202 | 1285.85     | 971.16      | 41.35 | 0.000            | 18.17            | $T_{ m L}$ |
| 440-Original Baseline       | 50  | -13.7200 | -9.8976  | 1301.54     | 968.76      | 39.94 | 0.000            | 18.07            | $T_{ m L}$ |
| 440-Original Baseline       | 51  | -13.7200 | -9.7750  | 1317.06     | 966.33      | 38.52 | 0.000            | 17.97            | $T_{ m L}$ |
| 440-Original Baseline       | 52  | -13.7200 | -9.6524  | 1332.42     | 963.87      | 37.11 | 0.000            | 17.87            | $T_{ m L}$ |
| 440-Original Baseline       | 53  | -13.7200 | -9.5298  | 1347.62     | 961.38      | 35.70 | 0.000            | 17.77            | $T_{ m L}$ |
| 440-Original Baseline       | 54  | -13.7200 | -9.4072  | 1362.66     | 958.87      | 34.29 | 0.000            | 17.67            | $T_{ m L}$ |
| 440-Original Baseline       | 55  | -13.7200 | -9.2846  | 1377.54     | 956.32      | 32.88 | 0.000            | 17.58            | $T_{ m L}$ |
| 440-Original Baseline       | 56  | -13.7200 | -9.1620  | 1392.27     | 953.76      | 31.48 | 0.000            | 17.48            | $T_{ m L}$ |
| 440-Original Baseline       | 57  | -13.7200 | -9.0394  | 1406.85     | 951.17      | 30.09 | 0.000            | 17.38            | $T_{ m L}$ |
| 440-Original Baseline       | 58  | -13.7200 | -8.9168  | 1421.29     | 948.56      | 28.70 | 0.000            | 17.28            | $T_{ m L}$ |
| 440-Original Baseline       | 59  | -13.7200 | -8.7942  | 1435.57     | 945.93      | 27.32 | 0.000            | 17.18            | $T_{ m L}$ |
| 440-Original Baseline       | 60  | -13.7200 | -8.6716  | 1449.72     | 943.28      | 25.95 | 0.000            | 17.08            | $T_{ m L}$ |
| 440-Original Baseline w CST | 25  | -13.6582 | -12.9530 | 815.54      | 990.44      | 74.27 | 0.770            | 20.59            | -          |
| 440-Original Baseline w CST | 26  | -13.6621 | -12.8300 | 835.41      | 991.90      | 73.06 | 0.801            | 20.49            | -          |
| 440-Original Baseline w CST | 27  | -13.6660 | -12.7070 | 854.97      | 993.33      | 71.84 | 0.832            | 20.39            | -          |
| 440-Original Baseline w CST | 28  | -13.6699 | -12.5840 | 874.25      | 994.72      | 70.61 | 0.863            | 20.30            | -          |
| 440-Original Baseline w CST | 29  | -13.6737 | -12.4610 | 893.24      | 996.04      | 69.38 | 0.893            | 20.20            | -          |
| 440-Original Baseline w CST | 30  | -13.6776 | -12.3380 | 911.97      | 997.28      | 68.13 | 0.924            | 20.10            | -          |
| 440-Original Baseline w CST | 31  | -13.6815 | -12.2150 | 930.43      | 998.39      | 66.88 | 0.955            | 20.01            | -          |
| 440-Original Baseline w CST | 32  | -13.6854 | -12.0920 | 948.64      | 999.35      | 65.61 | 0.986            | 19.91            | -          |
| 440-Original Baseline w CST | 33  | -13.6892 | -11.9690 | 966.60      | 1000.09     | 64.34 | 1.017            | 19.81            | -          |
| 440-Original Baseline w CST | 34  | -13.6931 | -11.8460 | 984.33      | 1000.58     | 63.06 | 1.048            | 19.72            | -          |
| 440-Original Baseline w CST | 35  | -13.6969 | -11.7231 | 1001.82     | 1000.79     | 61.77 | 1.078            | 19.62            | $T_{ m L}$ |
| 440-Original Baseline w CST | 36  | -13.7007 | -11.6001 | 1019.09     | 1000.69     | 60.47 | 1.109            | 19.52            | $T_{ m L}$ |
| 440-Original Baseline w CST | 37  | -13.7046 | -11.4771 | 1036.13     | 1000.30     | 59.16 | 1.140            | 19.43            | $T_{ m L}$ |
| 440-Original Baseline w CST | 38  | -13.7084 | -11.3541 | 1052.96     | 999.63      | 57.85 | 1.171            | 19.33            | $T_{ m L}$ |

| Category                    | WL  | B ∆Gp    | B ∆Gp    | $T_{\rm L}$ | $T_{ m L}$ | Visc       | TiO <sub>2</sub> | R <sub>2</sub> O | MAR        |
|-----------------------------|-----|----------|----------|-------------|------------|------------|------------------|------------------|------------|
|                             | (%) | MAR      | Value    | Pred        | MAR(°C)    | Pred       | wt%              | wt%              | Status     |
|                             |     |          |          | (°C)        | ,          | <b>(P)</b> |                  |                  |            |
| 440-Original Baseline w CST | 39  | -13.7122 | -11.2311 | 1069.58     | 998.73     | 56.53      | 1.202            | 19.23            | $T_{ m L}$ |
| 440-Original Baseline w CST | 40  | -13.7160 | -11.1081 | 1086.00     | 997.62     | 55.20      | 1.232            | 19.14            | $T_{ m L}$ |
| 440-Original Baseline w CST | 41  | -13.7198 | -10.9851 | 1102.21     | 996.36     | 53.86      | 1.263            | 19.04            | $T_{ m L}$ |
| 440-Original Baseline w CST | 42  | -13.7200 | -10.8621 | 1118.23     | 994.95     | 52.52      | 1.294            | 18.94            | $T_{ m L}$ |
| 440-Original Baseline w CST | 43  | -13.7200 | -10.7391 | 1134.06     | 993.44     | 51.17      | 1.325            | 18.85            | $T_{ m L}$ |
| 440-Original Baseline w CST | 44  | -13.7200 | -10.6161 | 1149.70     | 991.84     | 49.82      | 1.356            | 18.75            | $T_{ m L}$ |
| 440-Original Baseline w CST | 45  | -13.7200 | -10.4931 | 1165.15     | 990.15     | 48.46      | 1.386            | 18.65            | $T_{ m L}$ |
| 440-Original Baseline w CST | 46  | -13.7200 | -10.3701 | 1180.43     | 988.40     | 47.09      | 1.417            | 18.56            | $T_{ m L}$ |
| 440-Original Baseline w CST | 47  | -13.7200 | -10.2471 | 1195.53     | 986.60     | 45.72      | 1.448            | 18.46            | $T_{ m L}$ |
| 440-Original Baseline w CST | 48  | -13.7200 | -10.1241 | 1210.45     | 984.74     | 44.35      | 1.479            | 18.36            | $T_{ m L}$ |
| 440-Original Baseline w CST | 49  | -13.7200 | -10.0011 | 1225.21     | 982.84     | 42.97      | 1.510            | 18.27            | $T_{ m L}$ |
| 440-Original Baseline w CST | 50  | -13.7200 | -9.8781  | 1239.79     | 980.91     | 41.59      | 1.541            | 18.17            | $T_{ m L}$ |
| 440-Original Baseline w CST | 51  | -13.7200 | -9.7551  | 1254.22     | 978.93     | 40.21      | 1.571            | 18.07            | $T_{ m L}$ |
| 440-Original Baseline w CST | 52  | -13.7200 | -9.6321  | 1268.48     | 976.93     | 38.83      | 1.602            | 17.98            | $T_{ m L}$ |
| 440-Original Baseline w CST | 53  | -13.7200 | -9.5091  | 1282.58     | 974.90     | 37.45      | 1.633            | 17.88            | $T_{ m L}$ |
| 440-Original Baseline w CST | 54  | -13.7200 | -9.3861  | 1296.53     | 972.84     | 36.07      | 1.664            | 17.78            | $T_{ m L}$ |
| 440-Original Baseline w CST | 55  | -13.7200 | -9.2631  | 1310.32     | 970.75     | 34.69      | 1.695            | 17.69            | $T_{ m L}$ |
| 440-Original Baseline w CST | 56  | -13.7200 | -9.1402  | 1323.97     | 968.64     | 33.31      | 1.725            | 17.59            | $T_{ m L}$ |
| 440-Original Baseline w CST | 57  | -13.7200 | -9.0172  | 1337.47     | 966.52     | 31.94      | 1.756            | 17.49            | $T_{ m L}$ |
| 440-Original Baseline w CST | 58  | -13.7200 | -8.8942  | 1350.82     | 964.37     | 30.57      | 1.787            | 17.40            | $T_{ m L}$ |
| 440-Original Baseline w CST | 59  | -13.7200 | -8.7712  | 1364.02     | 962.21     | 29.21      | 1.818            | 17.30            | $T_{ m L}$ |
| 440-Original Baseline w CST | 60  | -13.7200 | -8.6482  | 1377.09     | 960.03     | 27.86      | 1.849            | 17.20            | $T_{ m L}$ |
| 320-SB4 Only Baseline       | 25  | -13.6886 | -12.8842 | 754.12      | 994.09     | 55.67      | 0.003            | 21.80            | -          |
| 320-SB4 Only Baseline       | 26  | -13.6876 | -12.8771 | 769.34      | 995.04     | 54.29      | 0.003            | 21.88            | -          |
| 320-SB4 Only Baseline       | 27  | -13.6865 | -12.8700 | 784.15      | 995.96     | 52.90      | 0.003            | 21.95            | -          |
| 320-SB4 Only Baseline       | 28  | -13.6854 | -12.8629 | 798.58      | 996.85     | 51.52      | 0.003            | 22.02            | -          |
| 320-SB4 Only Baseline       | 29  | -13.6843 | -12.8559 | 812.63      | 997.69     | 50.14      | 0.003            | 22.09            | -          |
| 320-SB4 Only Baseline       | 30  | -13.6832 | -12.8488 | 826.32      | 998.48     | 48.75      | 0.004            | 22.16            | -          |
| 320-SB4 Only Baseline       | 31  | -13.6821 | -12.8417 | 839.68      | 999.21     | 47.37      | 0.004            | 22.24            | -          |
| 320-SB4 Only Baseline       | 32  | -13.6810 | -12.8346 | 852.70      | 999.89     | 45.99      | 0.004            | 22.31            | -          |
| 320-SB4 Only Baseline       | 33  | -13.6799 | -12.8275 | 865.40      | 1000.49    | 44.61      | 0.004            | 22.38            | -          |
| 320-SB4 Only Baseline       | 34  | -13.6787 | -12.8204 | 877.80      | 1001.02    | 43.24      | 0.004            | 22.45            | -          |

| Category                    | WL  | BΔGp     | BΔGp     | $T_{\rm L}$  | T <sub>L</sub> | Visc        | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                    |
|-----------------------------|-----|----------|----------|--------------|----------------|-------------|------------------|------------------|------------------------|
|                             | (%) | MAR      | Value    | Pred<br>(°C) | MAR(°C)        | Pred<br>(P) | wt%              | wt%              | Status                 |
| 320-SB4 Only Baseline       | 35  | -13.6776 | -12.8133 | 889.90       | 1001.48        | 41.87       | 0.004            | 22.52            | -                      |
| 320-SB4 Only Baseline       | 36  | -13.6765 | -12.8063 | 901.71       | 1001.85        | 40.50       | 0.004            | 22.60            | -                      |
| 320-SB4 Only Baseline       | 37  | -13.6753 | -12.7992 | 913.25       | 1002.13        | 39.14       | 0.004            | 22.67            | -                      |
| 320-SB4 Only Baseline       | 38  | -13.6741 | -12.7921 | 924.52       | 1002.33        | 37.79       | 0.005            | 22.74            | -                      |
| 320-SB4 Only Baseline       | 39  | -13.6730 | -12.7850 | 935.54       | 1002.44        | 36.44       | 0.005            | 22.81            | -                      |
| 320-SB4 Only Baseline       | 40  | -13.6718 | -12.7779 | 946.31       | 1002.46        | 35.10       | 0.005            | 22.89            | -                      |
| 320-SB4 Only Baseline       | 41  | -13.6706 | -12.7708 | 956.83       | 1002.40        | 33.77       | 0.005            | 22.96            | -                      |
| 320-SB4 Only Baseline       | 42  | -13.6694 | -12.7638 | 967.13       | 1002.25        | 32.45       | 0.005            | 23.03            | -                      |
| 320-SB4 Only Baseline       | 43  | -13.6682 | -12.7567 | 977.19       | 1002.02        | 31.14       | 0.005            | 23.10            | -                      |
| 320-SB4 Only Baseline       | 44  | -13.6670 | -12.7496 | 987.04       | 1001.73        | 29.84       | 0.005            | 23.17            | -                      |
| 320-SB4 Only Baseline       | 45  | -13.6658 | -12.7425 | 996.67       | 1001.37        | 28.55       | 0.005            | 23.25            | -                      |
| 320-SB4 Only Baseline       | 46  | -13.6646 | -12.7354 | 1006.10      | 1000.94        | 27.28       | 0.006            | 23.32            | $T_{ m L}$             |
| 320-SB4 Only Baseline       | 47  | -13.6634 | -12.7283 | 1015.33      | 1000.47        | 26.02       | 0.006            | 23.39            | $T_{ m L}$             |
| 320-SB4 Only Baseline       | 48  | -13.6621 | -12.7212 | 1024.37      | 999.94         | 24.78       | 0.006            | 23.46            | $T_{ m L}$             |
| 320-SB4 Only Baseline       | 49  | -13.6609 | -12.7142 | 1033.22      | 999.38         | 23.55       | 0.006            | 23.53            | $T_L$ , low $\eta$     |
| 320-SB4 Only Baseline       | 50  | -13.6597 | -12.7071 | 1041.88      | 998.77         | 22.34       | 0.006            | 23.61            | $T_L$ , low $\eta$     |
| 320-SB4 Only Baseline       | 51  | -13.6584 | -12.7000 | 1050.37      | 998.14         | 21.16       | 0.006            | 23.68            | T <sub>L</sub> , low η |
| 320-SB4 Only Baseline       | 52  | -13.6571 | -12.6929 | 1058.69      | 997.47         | 19.99       | 0.006            | 23.75            | T <sub>L</sub> , low η |
| 320-SB4 Only Baseline       | 53  | -13.6559 | -12.6858 | 1066.84      | 996.79         | 18.84       | 0.006            | 23.82            | $T_L$ , low $\eta$     |
| 320-SB4 Only Baseline       | 54  | -13.6546 | -12.6787 | 1074.82      | 996.08         | 17.72       | 0.006            | 23.90            | $T_L$ , low $\eta$     |
| 320-SB4 Only Baseline       | 55  | -13.6533 | -12.6717 | 1082.65      | 995.35         | 16.62       | 0.007            | 23.97            | $T_L$ , low $\eta$     |
| 320-SB4 Only Baseline       | 56  | -13.6521 | -12.6646 | 1090.33      | 994.61         | 15.55       | 0.007            | 24.04            | $T_L$ , low $\eta$     |
| 320-SB4 Only Baseline       | 57  | -13.6508 | -12.6575 | 1097.85      | 993.85         | 14.50       | 0.007            | 24.11            | $T_L$ , low $\eta$     |
| 320-SB4 Only Baseline       | 58  | -13.6495 | -12.6504 | 1105.23      | 993.08         | 13.49       | 0.007            | 24.18            | T <sub>L</sub> , low η |
| 320-SB4 Only Baseline       | 59  | -13.6482 | -12.6433 | 1112.47      | 992.31         | 12.50       | 0.007            | 24.26            | $T_L$ , low $\eta$     |
| 320-SB4 Only Baseline       | 60  | -13.6469 | -12.6362 | 1119.56      | 991.53         | 11.55       | 0.007            | 24.33            | $T_L$ , low $\eta$     |
| 320-SB4 Only Baseline w CST | 25  | -13.6931 | -12.7412 | 743.69       | 994.03         | 56.67       | 0.488            | 21.61            | - L,                   |
| 320-SB4 Only Baseline w CST | 26  | -13.6922 | -12.7284 | 758.75       | 994.98         | 55.32       | 0.508            | 21.68            | -                      |
| 320-SB4 Only Baseline w CST | 27  | -13.6913 | -12.7156 | 773.41       | 995.90         | 53.97       | 0.527            | 21.74            | -                      |
| 320-SB4 Only Baseline w CST | 28  | -13.6904 | -12.7028 | 787.69       | 996.79         | 52.62       | 0.547            | 21.80            | -                      |
| 320-SB4 Only Baseline w CST | 29  | -13.6895 | -12.6900 | 801.60       | 997.64         | 51.26       | 0.566            | 21.87            | -                      |
| 320-SB4 Only Baseline w CST | 30  | -13.6886 | -12.6772 | 815.16       | 998.45         | 49.91       | 0.586            | 21.93            | -                      |

| Category                    | WL  | B ∆Gp    | B \( \Delta G p \) | $T_{ m L}$ | $T_{ m L}$ | Visc       | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                    |
|-----------------------------|-----|----------|--------------------|------------|------------|------------|------------------|------------------|------------------------|
|                             | (%) | MAR      | Value              | Pred       | MAR(°C)    | Pred       | wt%              | wt%              | Status                 |
|                             |     |          |                    | (°C)       |            | <b>(P)</b> |                  |                  |                        |
| 320-SB4 Only Baseline w CST | 31  | -13.6876 | -12.6644           | 828.39     | 999.22     | 48.56      | 0.605            | 22.00            | -                      |
| 320-SB4 Only Baseline w CST | 32  | -13.6867 | -12.6516           | 841.29     | 999.93     | 47.21      | 0.625            | 22.06            | -                      |
| 320-SB4 Only Baseline w CST | 33  | -13.6857 | -12.6388           | 853.88     | 1000.59    | 45.86      | 0.644            | 22.13            | -                      |
| 320-SB4 Only Baseline w CST | 34  | -13.6848 | -12.6260           | 866.17     | 1001.18    | 44.51      | 0.664            | 22.19            | -                      |
| 320-SB4 Only Baseline w CST | 35  | -13.6838 | -12.6132           | 878.16     | 1001.71    | 43.16      | 0.683            | 22.26            | -                      |
| 320-SB4 Only Baseline w CST | 36  | -13.6829 | -12.6004           | 889.88     | 1002.16    | 41.82      | 0.703            | 22.32            | -                      |
| 320-SB4 Only Baseline w CST | 37  | -13.6819 | -12.5876           | 901.32     | 1002.54    | 40.48      | 0.722            | 22.38            | -                      |
| 320-SB4 Only Baseline w CST | 38  | -13.6809 | -12.5748           | 912.50     | 1002.84    | 39.15      | 0.742            | 22.45            | -                      |
| 320-SB4 Only Baseline w CST | 39  | -13.6799 | -12.5619           | 923.43     | 1003.06    | 37.82      | 0.761            | 22.51            | -                      |
| 320-SB4 Only Baseline w CST | 40  | -13.6789 | -12.5491           | 934.11     | 1003.19    | 36.50      | 0.781            | 22.58            | -                      |
| 320-SB4 Only Baseline w CST | 41  | -13.6779 | -12.5363           | 944.56     | 1003.25    | 35.19      | 0.800            | 22.64            | -                      |
| 320-SB4 Only Baseline w CST | 42  | -13.6769 | -12.5235           | 954.77     | 1003.22    | 33.88      | 0.820            | 22.71            | -                      |
| 320-SB4 Only Baseline w CST | 43  | -13.6759 | -12.5107           | 964.76     | 1003.12    | 32.58      | 0.839            | 22.77            | -                      |
| 320-SB4 Only Baseline w CST | 44  | -13.6748 | -12.4979           | 974.54     | 1002.94    | 31.29      | 0.859            | 22.84            | -                      |
| 320-SB4 Only Baseline w CST | 45  | -13.6738 | -12.4851           | 984.10     | 1002.69    | 30.01      | 0.878            | 22.90            | -                      |
| 320-SB4 Only Baseline w CST | 46  | -13.6727 | -12.4723           | 993.46     | 1002.38    | 28.75      | 0.898            | 22.96            | -                      |
| 320-SB4 Only Baseline w CST | 47  | -13.6717 | -12.4595           | 1002.63    | 1002.01    | 27.49      | 0.917            | 23.03            | $T_{ m L}$             |
| 320-SB4 Only Baseline w CST | 48  | -13.6706 | -12.4467           | 1011.60    | 1001.59    | 26.25      | 0.937            | 23.09            | $T_{ m L}$             |
| 320-SB4 Only Baseline w CST | 49  | -13.6696 | -12.4339           | 1020.39    | 1001.12    | 25.03      | 0.956            | 23.16            | $T_{ m L}$             |
| 320-SB4 Only Baseline w CST | 50  | -13.6685 | -12.4211           | 1028.99    | 1000.60    | 23.81      | 0.976            | 23.22            | $T_L$ , low $\eta$     |
| 320-SB4 Only Baseline w CST | 51  | -13.6674 | -12.4083           | 1037.42    | 1000.05    | 22.62      | 0.996            | 23.29            | $T_L$ , low $\eta$     |
| 320-SB4 Only Baseline w CST | 52  | -13.6663 | -12.3955           | 1045.68    | 999.46     | 21.44      | 1.015            | 23.35            | T <sub>L</sub> , low η |
| 320-SB4 Only Baseline w CST | 53  | -13.6652 | -12.3827           | 1053.78    | 998.85     | 20.29      | 1.035            | 23.42            | T <sub>L</sub> , low η |
| 320-SB4 Only Baseline w CST | 54  | -13.6642 | -12.3699           | 1061.71    | 998.20     | 19.15      | 1.054            | 23.48            | $T_L$ , low $\eta$     |
| 320-SB4 Only Baseline w CST | 55  | -13.6630 | -12.3571           | 1069.48    | 997.54     | 18.04      | 1.074            | 23.54            | $T_L$ , low $\eta$     |
| 320-SB4 Only Baseline w CST | 56  | -13.6619 | -12.3443           | 1077.10    | 996.86     | 16.95      | 1.093            | 23.61            | $T_L$ , low $\eta$     |
| 320-SB4 Only Baseline w CST | 57  | -13.6608 | -12.3315           | 1084.58    | 996.16     | 15.88      | 1.113            | 23.67            | $T_L$ , low $\eta$     |
| 320-SB4 Only Baseline w CST | 58  | -13.6597 | -12.3187           | 1091.91    | 995.44     | 14.84      | 1.132            | 23.74            | $T_L$ , low $\eta$     |
| 320-SB4 Only Baseline w CST | 59  | -13.6586 | -12.3059           | 1099.09    | 994.72     | 13.83      | 1.152            | 23.80            | $T_L$ , low $\eta$     |
| 320-SB4 Only Baseline w CST | 60  | -13.6574 | -12.2931           | 1106.14    | 993.98     | 12.84      | 1.171            | 23.87            | $T_L$ , low $\eta$     |
| 418-SB4 Only Baseline       | 25  | -13.7200 | -10.1122           | 797.93     | 996.81     | 95.61      | 0.003            | 18.80            |                        |
| 418-SB4 Only Baseline       | 26  | -13.7200 | -10.1421           | 812.92     | 997.68     | 93.33      | 0.003            | 18.92            | _                      |

| Category              | WL  | B ∆Gp    | B ∆Gp    | $T_{ m L}$ | $T_{\rm L}$ | Visc       | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                |
|-----------------------|-----|----------|----------|------------|-------------|------------|------------------|------------------|--------------------|
|                       | (%) | MAR      | Value    | Pred       | MAR(°C)     | Pred       | wt%              | wt%              | Status             |
|                       |     |          |          | (°C)       |             | <b>(P)</b> |                  |                  |                    |
| 418-SB4 Only Baseline | 27  | -13.7200 | -10.1720 | 827.46     | 998.49      | 91.05      | 0.003            | 19.03            | -                  |
| 418-SB4 Only Baseline | 28  | -13.7200 | -10.2019 | 841.58     | 999.24      | 88.76      | 0.003            | 19.14            | -                  |
| 418-SB4 Only Baseline | 29  | -13.7200 | -10.2317 | 855.28     | 999.91      | 86.47      | 0.003            | 19.25            | -                  |
| 418-SB4 Only Baseline | 30  | -13.7200 | -10.2616 | 868.58     | 1000.51     | 84.17      | 0.004            | 19.36            | -                  |
| 418-SB4 Only Baseline | 31  | -13.7200 | -10.2915 | 881.52     | 1001.02     | 81.88      | 0.004            | 19.48            | -                  |
| 418-SB4 Only Baseline | 32  | -13.7200 | -10.3214 | 894.09     | 1001.44     | 79.59      | 0.004            | 19.59            | -                  |
| 418-SB4 Only Baseline | 33  | -13.7200 | -10.3512 | 906.31     | 1001.77     | 77.30      | 0.004            | 19.70            | -                  |
| 418-SB4 Only Baseline | 34  | -13.7200 | -10.3811 | 918.21     | 1002.00     | 75.01      | 0.004            | 19.81            | -                  |
| 418-SB4 Only Baseline | 35  | -13.7200 | -10.4110 | 929.78     | 1002.15     | 72.73      | 0.004            | 19.92            | -                  |
| 418-SB4 Only Baseline | 36  | -13.7200 | -10.4409 | 941.05     | 1002.20     | 70.45      | 0.004            | 20.04            | -                  |
| 418-SB4 Only Baseline | 37  | -13.7200 | -10.4707 | 952.03     | 1002.16     | 68.18      | 0.004            | 20.15            | -                  |
| 418-SB4 Only Baseline | 38  | -13.7200 | -10.5006 | 962.72     | 1002.03     | 65.91      | 0.005            | 20.26            | -                  |
| 418-SB4 Only Baseline | 39  | -13.7200 | -10.5305 | 973.14     | 1001.83     | 63.65      | 0.005            | 20.37            | -                  |
| 418-SB4 Only Baseline | 40  | -13.7200 | -10.5604 | 983.30     | 1001.55     | 61.41      | 0.005            | 20.49            | -                  |
| 418-SB4 Only Baseline | 41  | -13.7200 | -10.5902 | 993.20     | 1001.20     | 59.17      | 0.005            | 20.60            | -                  |
| 418-SB4 Only Baseline | 42  | -13.7200 | -10.6201 | 1002.86    | 1000.79     | 56.94      | 0.005            | 20.71            | $T_{ m L}$         |
| 418-SB4 Only Baseline | 43  | -13.7200 | -10.6500 | 1012.28    | 1000.33     | 54.73      | 0.005            | 20.82            | $T_{ m L}$         |
| 418-SB4 Only Baseline | 44  | -13.7200 | -10.6799 | 1021.48    | 999.82      | 52.53      | 0.005            | 20.93            | $T_{ m L}$         |
| 418-SB4 Only Baseline | 45  | -13.7200 | -10.7097 | 1030.46    | 999.26      | 50.36      | 0.005            | 21.05            | $T_{\rm L}$        |
| 418-SB4 Only Baseline | 46  | -13.7200 | -10.7396 | 1039.22    | 998.67      | 48.20      | 0.006            | 21.16            | $T_{\rm L}$        |
| 418-SB4 Only Baseline | 47  | -13.7200 | -10.7695 | 1047.78    | 998.05      | 46.06      | 0.006            | 21.27            | $T_{\rm L}$        |
| 418-SB4 Only Baseline | 48  | -13.7200 | -10.7994 | 1056.14    | 997.40      | 43.94      | 0.006            | 21.38            | $T_{\rm L}$        |
| 418-SB4 Only Baseline | 49  | -13.7200 | -10.8292 | 1064.31    | 996.73      | 41.85      | 0.006            | 21.49            | $T_{\rm L}$        |
| 418-SB4 Only Baseline | 50  | -13.7200 | -10.8591 | 1072.29    | 996.04      | 39.78      | 0.006            | 21.61            | $T_{\rm L}$        |
| 418-SB4 Only Baseline | 51  | -13.7200 | -10.8890 | 1080.09    | 995.33      | 37.74      | 0.006            | 21.72            | $T_{\rm L}$        |
| 418-SB4 Only Baseline | 52  | -13.7200 | -10.9189 | 1087.72    | 994.61      | 35.74      | 0.006            | 21.83            | $T_{\rm L}$        |
| 418-SB4 Only Baseline | 53  | -13.7200 | -10.9487 | 1095.19    | 993.87      | 33.76      | 0.006            | 21.94            | $T_{ m L}$         |
| 418-SB4 Only Baseline | 54  | -13.7180 | -10.9786 | 1102.48    | 993.13      | 31.83      | 0.006            | 22.06            | $T_{ m L}$         |
| 418-SB4 Only Baseline | 55  | -13.7153 | -11.0085 | 1109.62    | 992.38      | 29.92      | 0.007            | 22.17            | $T_{ m L}$         |
| 418-SB4 Only Baseline | 56  | -13.7126 | -11.0384 | 1116.61    | 991.63      | 28.06      | 0.007            | 22.28            | $T_{ m L}$         |
| 418-SB4 Only Baseline | 57  | -13.7099 | -11.0682 | 1123.45    | 990.87      | 26.25      | 0.007            | 22.39            | $T_{ m L}$         |
| 418-SB4 Only Baseline | 58  | -13.7072 | -11.0981 | 1130.14    | 990.11      | 24.47      | 0.007            | 22.50            | $T_L$ , low $\eta$ |

| Category                    | WL  | B ∆Gp    | B ∆Gp    | $T_{ m L}$ | $T_{\rm L}$ | Visc       | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                |
|-----------------------------|-----|----------|----------|------------|-------------|------------|------------------|------------------|--------------------|
|                             | (%) | MAR      | Value    | Pred       | MAR(°C)     | Pred       | wt%              | wt%              | Status             |
|                             |     |          |          | (°C)       |             | <b>(P)</b> |                  |                  |                    |
| 418-SB4 Only Baseline       | 59  | -13.7045 | -11.1280 | 1136.69    | 989.35      | 22.75      | 0.007            | 22.62            | $T_L$ , low $\eta$ |
| 418-SB4 Only Baseline       | 60  | -13.7017 | -11.1579 | 1143.11    | 988.58      | 21.07      | 0.007            | 22.73            | $T_L$ , low $\eta$ |
| 418-SB4 Only Baseline w CST | 25  | -13.7200 | -9.9692  | 787.30     | 996.80      | 97.01      | 0.488            | 18.61            | -                  |
| 418-SB4 Only Baseline w CST | 26  | -13.7200 | -9.9934  | 802.14     | 997.69      | 94.78      | 0.508            | 18.72            | -                  |
| 418-SB4 Only Baseline w CST | 27  | -13.7200 | -10.0176 | 816.54     | 998.53      | 92.54      | 0.527            | 18.82            | -                  |
| 418-SB4 Only Baseline w CST | 28  | -13.7200 | -10.0417 | 830.51     | 999.30      | 90.30      | 0.547            | 18.92            | -                  |
| 418-SB4 Only Baseline w CST | 29  | -13.7200 | -10.0659 | 844.09     | 1000.02     | 88.06      | 0.566            | 19.03            | -                  |
| 418-SB4 Only Baseline w CST | 30  | -13.7200 | -10.0900 | 857.27     | 1000.67     | 85.81      | 0.586            | 19.13            | -                  |
| 418-SB4 Only Baseline w CST | 31  | -13.7200 | -10.1142 | 870.09     | 1001.25     | 83.57      | 0.605            | 19.24            | -                  |
| 418-SB4 Only Baseline w CST | 32  | -13.7200 | -10.1383 | 882.55     | 1001.75     | 81.32      | 0.625            | 19.34            | -                  |
| 418-SB4 Only Baseline w CST | 33  | -13.7200 | -10.1625 | 894.67     | 1002.17     | 79.07      | 0.644            | 19.45            | -                  |
| 418-SB4 Only Baseline w CST | 34  | -13.7200 | -10.1866 | 906.46     | 1002.50     | 76.82      | 0.664            | 19.55            | -                  |
| 418-SB4 Only Baseline w CST | 35  | -13.7200 | -10.2108 | 917.94     | 1002.75     | 74.58      | 0.683            | 19.66            | -                  |
| 418-SB4 Only Baseline w CST | 36  | -13.7200 | -10.2350 | 929.11     | 1002.92     | 72.34      | 0.703            | 19.76            | -                  |
| 418-SB4 Only Baseline w CST | 37  | -13.7200 | -10.2591 | 940.00     | 1002.99     | 70.10      | 0.722            | 19.86            | -                  |
| 418-SB4 Only Baseline w CST | 38  | -13.7200 | -10.2833 | 950.61     | 1002.99     | 67.87      | 0.742            | 19.97            | -                  |
| 418-SB4 Only Baseline w CST | 39  | -13.7200 | -10.3074 | 960.94     | 1002.90     | 65.64      | 0.761            | 20.07            | -                  |
| 418-SB4 Only Baseline w CST | 40  | -13.7200 | -10.3316 | 971.02     | 1002.73     | 63.42      | 0.781            | 20.18            | -                  |
| 418-SB4 Only Baseline w CST | 41  | -13.7200 | -10.3557 | 980.85     | 1002.50     | 61.21      | 0.800            | 20.28            | -                  |
| 418-SB4 Only Baseline w CST | 42  | -13.7200 | -10.3799 | 990.43     | 1002.20     | 59.01      | 0.820            | 20.39            | -                  |
| 418-SB4 Only Baseline w CST | 43  | -13.7200 | -10.4040 | 999.78     | 1001.84     | 56.83      | 0.839            | 20.49            | -                  |
| 418-SB4 Only Baseline w CST | 44  | -13.7200 | -10.4282 | 1008.91    | 1001.43     | 54.65      | 0.859            | 20.60            | $T_{ m L}$         |
| 418-SB4 Only Baseline w CST | 45  | -13.7200 | -10.4524 | 1017.82    | 1000.97     | 52.49      | 0.878            | 20.70            | $T_{ m L}$         |
| 418-SB4 Only Baseline w CST | 46  | -13.7200 | -10.4765 | 1026.52    | 1000.46     | 50.34      | 0.898            | 20.80            | $T_{ m L}$         |
| 418-SB4 Only Baseline w CST | 47  | -13.7200 | -10.5007 | 1035.01    | 999.92      | 48.22      | 0.917            | 20.91            | $T_{ m L}$         |
| 418-SB4 Only Baseline w CST | 48  | -13.7200 | -10.5248 | 1043.31    | 999.35      | 46.11      | 0.937            | 21.01            | $T_{ m L}$         |
| 418-SB4 Only Baseline w CST | 49  | -13.7200 | -10.5490 | 1051.42    | 998.75      | 44.02      | 0.956            | 21.12            | $T_{ m L}$         |
| 418-SB4 Only Baseline w CST | 50  | -13.7200 | -10.5731 | 1059.35    | 998.13      | 41.96      | 0.976            | 21.22            | $T_{ m L}$         |
| 418-SB4 Only Baseline w CST | 51  | -13.7200 | -10.5973 | 1067.09    | 997.48      | 39.92      | 0.996            | 21.33            | $T_{\mathrm{L}}$   |
| 418-SB4 Only Baseline w CST | 52  | -13.7200 | -10.6214 | 1074.67    | 996.82      | 37.91      | 1.015            | 21.43            | $T_{ m L}$         |
| 418-SB4 Only Baseline w CST | 53  | -13.7200 | -10.6456 | 1082.07    | 996.14      | 35.93      | 1.035            | 21.54            | $T_{ m L}$         |
| 418-SB4 Only Baseline w CST | 54  | -13.7200 | -10.6698 | 1089.32    | 995.45      | 33.97      | 1.054            | 21.64            | $T_{ m L}$         |

| Category                    | WL  | B ∆Gp    | B \( \Delta G p \) | $T_{\rm L}$ | $T_{ m L}$ | Visc       | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                    |
|-----------------------------|-----|----------|--------------------|-------------|------------|------------|------------------|------------------|------------------------|
|                             | (%) | MAR      | Value              | Pred        | MAR(°C)    | Pred       | wt%              | wt%              | Status                 |
|                             |     |          |                    | (°C)        |            | <b>(P)</b> |                  |                  |                        |
| 418-SB4 Only Baseline w CST | 55  | -13.7200 | -10.6939           | 1096.41     | 994.76     | 32.06      | 1.074            | 21.74            | $T_{\rm L}$            |
| 418-SB4 Only Baseline w CST | 56  | -13.7200 | -10.7181           | 1103.34     | 994.05     | 30.18      | 1.093            | 21.85            | $T_{ m L}$             |
| 418-SB4 Only Baseline w CST | 57  | -13.7199 | -10.7422           | 1110.13     | 993.33     | 28.33      | 1.113            | 21.95            | $T_{L}$                |
| 418-SB4 Only Baseline w CST | 58  | -13.7174 | -10.7664           | 1116.77     | 992.61     | 26.53      | 1.132            | 22.06            | $T_{ m L}$             |
| 418-SB4 Only Baseline w CST | 59  | -13.7148 | -10.7905           | 1123.28     | 991.89     | 24.77      | 1.152            | 22.16            | $T_L$ , low $\eta$     |
| 418-SB4 Only Baseline w CST | 60  | -13.7123 | -10.8147           | 1129.65     | 991.16     | 23.06      | 1.171            | 22.27            | T <sub>L</sub> , low η |
| 440-SB4 Only Baseline       | 25  | -13.5747 | -15.1091           | 723.07      | 989.74     | 62.08      | 0.003            | 24.05            | $\Delta G_{ m P}$      |
| 440-SB4 Only Baseline       | 26  | -13.5752 | -15.0724           | 738.13      | 990.64     | 60.47      | 0.003            | 24.10            | $\Delta G_{ m P}$      |
| 440-SB4 Only Baseline       | 27  | -13.5757 | -15.0356           | 752.82      | 991.52     | 58.87      | 0.003            | 24.14            | $\Delta G_{ m P}$      |
| 440-SB4 Only Baseline       | 28  | -13.5762 | -14.9989           | 767.16      | 992.37     | 57.27      | 0.003            | 24.18            | $\Delta G_{ m P}$      |
| 440-SB4 Only Baseline       | 29  | -13.5768 | -14.9621           | 781.16      | 993.20     | 55.66      | 0.003            | 24.22            | $\Delta G_{ m P}$      |
| 440-SB4 Only Baseline       | 30  | -13.5773 | -14.9254           | 794.83      | 993.99     | 54.07      | 0.004            | 24.26            | $\Delta G_{ m P}$      |
| 440-SB4 Only Baseline       | 31  | -13.5777 | -14.8886           | 808.19      | 994.75     | 52.47      | 0.004            | 24.31            | $\Delta G_{ m P}$      |
| 440-SB4 Only Baseline       | 32  | -13.5782 | -14.8519           | 821.25      | 995.47     | 50.88      | 0.004            | 24.35            | $\Delta G_{ m P}$      |
| 440-SB4 Only Baseline       | 33  | -13.5787 | -14.8151           | 834.02      | 996.14     | 49.30      | 0.004            | 24.39            | $\Delta G_{ m P}$      |
| 440-SB4 Only Baseline       | 34  | -13.5792 | -14.7784           | 846.51      | 996.76     | 47.72      | 0.004            | 24.43            | $\Delta G_{ m P}$      |
| 440-SB4 Only Baseline       | 35  | -13.5796 | -14.7416           | 858.73      | 997.33     | 46.15      | 0.004            | 24.47            | $\Delta G_{ m P}$      |
| 440-SB4 Only Baseline       | 36  | -13.5801 | -14.7049           | 870.69      | 997.84     | 44.58      | 0.004            | 24.52            | $\Delta G_{ m P}$      |
| 440-SB4 Only Baseline       | 37  | -13.5805 | -14.6681           | 882.40      | 998.29     | 43.02      | 0.004            | 24.56            | $\Delta G_{ m P}$      |
| 440-SB4 Only Baseline       | 38  | -13.5809 | -14.6314           | 893.86      | 998.68     | 41.48      | 0.005            | 24.60            | $\Delta G_{ m P}$      |
| 440-SB4 Only Baseline       | 39  | -13.5814 | -14.5946           | 905.09      | 999.00     | 39.94      | 0.005            | 24.64            | $\Delta G_{ m P}$      |
| 440-SB4 Only Baseline       | 40  | -13.5818 | -14.5579           | 916.08      | 999.25     | 38.41      | 0.005            | 24.69            | $\Delta G_{ m P}$      |
| 440-SB4 Only Baseline       | 41  | -13.5822 | -14.5211           | 926.86      | 999.42     | 36.90      | 0.005            | 24.73            | $\Delta G_{P}$         |
| 440-SB4 Only Baseline       | 42  | -13.5826 | -14.4844           | 937.43      | 999.53     | 35.40      | 0.005            | 24.77            | $\Delta G_{P}$         |
| 440-SB4 Only Baseline       | 43  | -13.5830 | -14.4476           | 947.78      | 999.57     | 33.91      | 0.005            | 24.81            | $\Delta G_{P}$         |
| 440-SB4 Only Baseline       | 44  | -13.5833 | -14.4109           | 957.93      | 999.54     | 32.44      | 0.005            | 24.85            | $\Delta G_{P}$         |
| 440-SB4 Only Baseline       | 45  | -13.5837 | -14.3741           | 967.89      | 999.44     | 30.99      | 0.005            | 24.90            | $\Delta G_{P}$         |
| 440-SB4 Only Baseline       | 46  | -13.5841 | -14.3374           | 977.66      | 999.27     | 29.55      | 0.006            | 24.94            | $\Delta G_{P}$         |
| 440-SB4 Only Baseline       | 47  | -13.5844 | -14.3006           | 987.24      | 999.04     | 28.14      | 0.006            | 24.98            | $\Delta G_{P}$         |
| 440-SB4 Only Baseline       | 48  | -13.5848 | -14.2639           | 996.64      | 998.76     | 26.74      | 0.006            | 25.02            | $\Delta G_{P}$         |
| 440-SB4 Only Baseline       | 49  | -13.5851 | -14.2271           | 1005.87     | 998.42     | 25.37      | 0.006            | 25.06            | $\Delta G_P, T_L$      |

| Category   | WL  | B ∆Gp    | B \( \Delta G p \) | $T_{ m L}$ | $T_{\rm L}$ | Visc  | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                                 |
|--|-----|----------|--------------------|------------|-------------|-------|------------------|------------------|-------------------------------------|
|  | (%) | MAR      | Value              | Pred       | MAR(°C)     | Pred  | wt%              | wt%              | Status                              |
|  |     |          |                    | (°C)       |             | (P)   |                  |                  |                                     |
| 440-SB4 Only Baseline  | 50  | -13.5854 | -14.1904           | 1014.93    | 998.03      | 24.02 | 0.006            | 25.11            | $\Delta G_P$ , $T_L$ , low          |
|  |     |          |                    | 1000       | 227.52      |       | 0.005            |                  | η                                   |
| 440-SB4 Only Baseline  | 51  | -13.5858 | -14.1536           | 1023.83    | 997.60      | 22.69 | 0.006            | 25.15            | $\Delta G_P, T_L$ , low             |
| 440 GD 4 G 1 D 1   |     | 12.5061  | 111160             | 1000 56    | 007.10      | 21.20 | 0.006            | 07.10            | η                                   |
| 440-SB4 Only Baseline  | 52  | -13.5861 | -14.1169           | 1032.56    | 997.12      | 21.39 | 0.006            | 25.19            | $\Delta G_P, T_L$ , low             |
| 440 SD4 Only Descline  | 53  | 12 5064  | -14.0801           | 1041 12    | 996.60      | 20.12 | 0.006            | 25.23            | η                                   |
| 440-SB4 Only Baseline  | 33  | -13.5864 | -14.0801           | 1041.13    | 990.00      | 20.12 | 0.006            | 25.25            | $\Delta G_P, T_L, low$              |
| 440-SB4 Only Baseline  | 54  | -13.5866 | -14.0434           | 1049.56    | 996.05      | 18.87 | 0.006            | 25.28            | $\frac{\eta}{\Delta G_P, T_L, low}$ |
| 440-3B4 Only Baseline  | 34  | -13.3600 | -14.0434           | 1049.30    | 990.03      | 10.07 | 0.000            | 23.26            | ΔOp, IL, IOW                        |
| 440-SB4 Only Baseline  | 55  | -13.5869 | -14.0066           | 1057.84    | 995.47      | 17.66 | 0.007            | 25.32            | $\Delta G_P, T_L, low$              |
| 440-3B4 Only Baseline  | 33  | -13.3007 | -14.0000           | 1037.04    | 773.47      | 17.00 | 0.007            | 23.32            | ΔGP, IL, IOW                        |
| 440-SB4 Only Baseline  | 56  | -13.5872 | -13.9699           | 1065.97    | 994.86      | 16.48 | 0.007            | 25.36            | $\Delta G_P, T_L, low$              |
| 110 SB 1 Only Busenine   | 30  | 13.5072  | 13.7077            | 1003.57    | 771.00      | 10.10 | 0.007            | 23.30            | n                                   |
| 440-SB4 Only Baseline  | 57  | -13.5875 | -13.9331           | 1073.96    | 994.22      | 15.33 | 0.007            | 25.40            | $\Delta G_P, T_L, low$              |
|  |     |          |                    |            | ,,          |       |                  |                  | n                                   |
| 440-SB4 Only Baseline  | 58  | -13.5877 | -13.8964           | 1081.81    | 993.56      | 14.21 | 0.007            | 25.44            | $\Delta G_P, T_L, low$              |
| , and the second |     |          |                    |            |             |       |                  |                  | η                                   |
| 440-SB4 Only Baseline  | 59  | -13.5880 | -13.8596           | 1089.53    | 992.88      | 13.14 | 0.007            | 25.49            | $\Delta G_P, T_L$ , low             |
|  |     |          |                    |            |             |       |                  |                  | η                                   |
| 440-SB4 Only Baseline  | 60  | -13.5882 | -13.8229           | 1097.12    | 992.19      | 12.10 | 0.007            | 25.53            | $\Delta G_P$ , $T_L$ , low          |
|  |     |          |                    |            |             |       |                  |                  | η                                   |
| 440-SB4 Only Baseline w CST  | 25  | -13.5788 | -14.9661           | 712.72     | 989.62      | 63.20 | 0.488            | 23.86            | $\Delta G_{P}$                      |
| 440-SB4 Only Baseline w CST  | 26  | -13.5795 | -14.9237           | 727.61     | 990.50      | 61.63 | 0.508            | 23.90            | $\Delta G_{P}$                      |
| 440-SB4 Only Baseline w CST  | 27  | -13.5802 | -14.8812           | 742.13     | 991.36      | 60.07 | 0.527            | 23.93            | $\Delta G_{P}$                      |
| 440-SB4 Only Baseline w CST  | 28  | -13.5809 | -14.8387           | 756.31     | 992.19      | 58.50 | 0.547            | 23.96            | $\Delta G_{P}$                      |
| 440-SB4 Only Baseline w CST  | 29  | -13.5816 | -14.7963           | 770.16     | 993.01      | 56.93 | 0.566            | 24.00            | $\Delta G_{ m P}$                   |
| 440-SB4 Only Baseline w CST  | 30  | -13.5822 | -14.7538           | 783.68     | 993.79      | 55.37 | 0.586            | 24.03            | $\Delta G_{P}$                      |
| 440-SB4 Only Baseline w CST  | 31  | -13.5829 | -14.7113           | 796.90     | 994.55      | 53.80 | 0.605            | 24.07            | $\Delta G_{P}$                      |
| 440-SB4 Only Baseline w CST  | 32  | -13.5835 | -14.6689           | 809.83     | 995.27      | 52.24 | 0.625            | 24.10            | $\Delta G_{P}$                      |
| 440-SB4 Only Baseline w CST  | 33  | -13.5842 | -14.6264           | 822.47     | 995.95      | 50.69 | 0.644            | 24.14            | $\Delta G_{P}$                      |
| 440-SB4 Only Baseline w CST  | 34  | -13.5848 | -14.5839           | 834.84     | 996.59      | 49.14 | 0.664            | 24.17            | $\Delta G_{P}$                      |

| Category                    | WL  | B ∆Gp    | B ∆Gp    | $T_{ m L}$ | $T_{ m L}$ | Visc       | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                                 |
|-----------------------------|-----|----------|----------|------------|------------|------------|------------------|------------------|-------------------------------------|
|                             | (%) | MAR      | Value    | Pred       | MAR(°C)    | Pred       | wt%              | wt%              | Status                              |
|                             |     |          |          | (°C)       | , ,        | <b>(P)</b> |                  |                  |                                     |
| 440-SB4 Only Baseline w CST | 35  | -13.5855 | -14.5414 | 846.94     | 997.19     | 47.59      | 0.683            | 24.21            | $\Delta G_{ m P}$                   |
| 440-SB4 Only Baseline w CST | 36  | -13.5861 | -14.4990 | 858.79     | 997.73     | 46.05      | 0.703            | 24.24            | $\Delta G_{	ext{P}}$                |
| 440-SB4 Only Baseline w CST | 37  | -13.5867 | -14.4565 | 870.38     | 998.23     | 44.52      | 0.722            | 24.27            | $\Delta G_{	ext{P}}$                |
| 440-SB4 Only Baseline w CST | 38  | -13.5873 | -14.4140 | 881.74     | 998.66     | 42.99      | 0.742            | 24.31            | $\Delta G_{P}$                      |
| 440-SB4 Only Baseline w CST | 39  | -13.5879 | -14.3716 | 892.87     | 999.04     | 41.48      | 0.761            | 24.34            | $\Delta G_{	ext{P}}$                |
| 440-SB4 Only Baseline w CST | 40  | -13.5885 | -14.3291 | 903.77     | 999.36     | 39.97      | 0.781            | 24.38            | $\Delta G_{ m P}$                   |
| 440-SB4 Only Baseline w CST | 41  | -13.5891 | -14.2866 | 914.46     | 999.61     | 38.47      | 0.800            | 24.41            | $\Delta G_{ m P}$                   |
| 440-SB4 Only Baseline w CST | 42  | -13.5896 | -14.2442 | 924.93     | 999.80     | 36.99      | 0.820            | 24.45            | $\Delta G_{	ext{P}}$                |
| 440-SB4 Only Baseline w CST | 43  | -13.5902 | -14.2017 | 935.20     | 999.93     | 35.51      | 0.839            | 24.48            | $\Delta G_{ m P}$                   |
| 440-SB4 Only Baseline w CST | 44  | -13.5907 | -14.1592 | 945.27     | 999.99     | 34.05      | 0.859            | 24.52            | $\Delta G_{ m P}$                   |
| 440-SB4 Only Baseline w CST | 45  | -13.5913 | -14.1167 | 955.15     | 999.99     | 32.61      | 0.878            | 24.55            | $\Delta G_{ m P}$                   |
| 440-SB4 Only Baseline w CST | 46  | -13.5918 | -14.0743 | 964.84     | 999.92     | 31.18      | 0.898            | 24.58            | $\Delta G_{ m P}$                   |
| 440-SB4 Only Baseline w CST | 47  | -13.5923 | -14.0318 | 974.35     | 999.79     | 29.76      | 0.917            | 24.62            | $\Delta G_{ m P}$                   |
| 440-SB4 Only Baseline w CST | 48  | -13.5929 | -13.9893 | 983.68     | 999.61     | 28.37      | 0.937            | 24.65            | $\Delta G_{ m P}$                   |
| 440-SB4 Only Baseline w CST | 49  | -13.5934 | -13.9469 | 992.84     | 999.37     | 26.99      | 0.956            | 24.69            | $\Delta G_{ m P}$                   |
| 440-SB4 Only Baseline w CST | 50  | -13.5939 | -13.9044 | 1001.83    | 999.08     | 25.63      | 0.976            | 24.72            | $\Delta G_P, T_L$                   |
| 440-SB4 Only Baseline w CST | 51  | -13.5944 | -13.8619 | 1010.66    | 998.74     | 24.30      | 0.996            | 24.76            | $\Delta G_P$ , $T_L$ , low          |
|                             |     |          |          |            |            |            |                  |                  | η                                   |
| 440-SB4 Only Baseline w CST | 52  | -13.5948 | -13.8195 | 1019.33    | 998.36     | 22.99      | 1.015            | 24.79            | $\Delta G_P, T_L$ , low             |
|                             |     |          |          |            |            |            |                  |                  |                                     |
| 440-SB4 Only Baseline w CST | 53  | -13.5953 | -13.7770 | 1027.84    | 997.93     | 21.70      | 1.035            | 24.83            | $\Delta G_P, T_L, low$              |
|                             |     |          |          |            |            |            |                  |                  | η                                   |
| 440-SB4 Only Baseline w CST | 54  | -13.5958 | -13.7345 | 1036.21    | 997.47     | 20.44      | 1.054            | 24.86            | $\Delta G_P, T_L$ , low             |
|                             |     |          |          |            |            |            |                  |                  | η                                   |
| 440-SB4 Only Baseline w CST | 55  | -13.5962 | -13.6920 | 1044.43    | 996.97     | 19.20      | 1.074            | 24.89            | $\Delta G_P$ , $T_L$ , low          |
|                             |     |          |          |            |            |            |                  |                  | η                                   |
| 440-SB4 Only Baseline w CST | 56  | -13.5967 | -13.6496 | 1052.50    | 996.44     | 18.00      | 1.093            | 24.93            | $\Delta G_P, T_L$ , low             |
|                             |     |          |          |            |            |            |                  |                  | η                                   |
| 440-SB4 Only Baseline w CST | 57  | -13.5971 | -13.6071 | 1060.44    | 995.88     | 16.82      | 1.113            | 24.96            | $\Delta G_P$ , $T_L$ , low          |
| -                           |     |          |          |            |            |            |                  |                  |                                     |
| 440-SB4 Only Baseline w CST | 58  | -13.5976 | -13.5646 | 1068.24    | 995.30     | 15.68      | 1.132            | 25.00            | $\frac{\eta}{\Delta G_P, T_L, low}$ |
| -                           |     |          |          |            |            |            |                  |                  | η                                   |

| Category                    | WL  | B \( \Delta G p \) | B ΔGp    | $T_{ m L}$ | $T_{ m L}$ | Visc  | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                        |
|-----------------------------|-----|--------------------|----------|------------|------------|-------|------------------|------------------|----------------------------|
|                             | (%) | MAR                | Value    | Pred       | MAR(°C)    | Pred  | wt%              | wt%              | Status                     |
|                             |     |                    |          | (°C)       |            | (P)   |                  |                  |                            |
| 440-SB4 Only Baseline w CST | 59  | -13.5980           | -13.5222 | 1075.91    | 994.69     | 14.57 | 1.152            | 25.03            | $\Delta G_P$ , $T_L$ , low |
|                             |     |                    |          |            |            |       |                  |                  | η                          |
| 440-SB4 Only Baseline w CST | 60  | -13.5984           | -13.4797 | 1083.45    | 994.07     | 13.49 | 1.171            | 25.07            | $\Delta G_P, T_L$ , low    |
|                             |     |                    |          |            |            |       |                  |                  | η                          |
| 320-1100 Eq Baseline        | 25  | -13.7073           | -12.4602 | 759.04     | 997.41     | 52.96 | 0.006            | 20.52            | -                          |
| 320-1100 Eq Baseline        | 26  | -13.7070           | -12.4362 | 775.17     | 999.65     | 51.51 | 0.006            | 20.54            | -                          |
| 320-1100 Eq Baseline        | 27  | -13.7067           | -12.4122 | 790.93     | 1001.77    | 50.06 | 0.006            | 20.57            | -                          |
| 320-1100 Eq Baseline        | 28  | -13.7064           | -12.3881 | 806.32     | 1003.11    | 48.61 | 0.006            | 20.59            | -                          |
| 320-1100 Eq Baseline        | 29  | -13.7061           | -12.3641 | 821.38     | 1004.17    | 47.18 | 0.006            | 20.61            | -                          |
| 320-1100 Eq Baseline        | 30  | -13.7058           | -12.3400 | 836.10     | 1005.19    | 45.74 | 0.007            | 20.63            | -                          |
| 320-1100 Eq Baseline        | 31  | -13.7055           | -12.3160 | 850.50     | 1006.16    | 44.32 | 0.007            | 20.65            | -                          |
| 320-1100 Eq Baseline        | 32  | -13.7052           | -12.2920 | 864.59     | 1007.08    | 42.90 | 0.007            | 20.67            | -                          |
| 320-1100 Eq Baseline        | 33  | -13.7049           | -12.2679 | 878.39     | 1007.93    | 41.48 | 0.007            | 20.69            | -                          |
| 320-1100 Eq Baseline        | 34  | -13.7045           | -12.2439 | 891.90     | 1008.71    | 40.08 | 0.007            | 20.71            | -                          |
| 320-1100 Eq Baseline        | 35  | -13.7042           | -12.2198 | 905.14     | 1009.40    | 38.68 | 0.008            | 20.73            | -                          |
| 320-1100 Eq Baseline        | 36  | -13.7039           | -12.1958 | 918.10     | 1009.99    | 37.30 | 0.008            | 20.75            | -                          |
| 320-1100 Eq Baseline        | 37  | -13.7035           | -12.1717 | 930.81     | 1010.47    | 35.92 | 0.008            | 20.78            | -                          |
| 320-1100 Eq Baseline        | 38  | -13.7032           | -12.1477 | 943.26     | 1010.83    | 34.56 | 0.008            | 20.80            | -                          |
| 320-1100 Eq Baseline        | 39  | -13.7028           | -12.1237 | 955.47     | 1011.06    | 33.21 | 0.009            | 20.82            | -                          |
| 320-1100 Eq Baseline        | 40  | -13.7025           | -12.0996 | 967.45     | 1011.15    | 31.87 | 0.009            | 20.84            | -                          |
| 320-1100 Eq Baseline        | 41  | -13.7021           | -12.0756 | 979.19     | 1011.12    | 30.54 | 0.009            | 20.86            | -                          |
| 320-1100 Eq Baseline        | 42  | -13.7017           | -12.0515 | 990.71     | 1010.96    | 29.23 | 0.009            | 20.88            | -                          |
| 320-1100 Eq Baseline        | 43  | -13.7014           | -12.0275 | 1002.01    | 1010.67    | 27.94 | 0.009            | 20.90            | -                          |
| 320-1100 Eq Baseline        | 44  | -13.7010           | -12.0034 | 1013.11    | 1010.28    | 26.66 | 0.010            | 20.92            | $T_{\rm L}$                |
| 320-1100 Eq Baseline        | 45  | -13.7006           | -11.9794 | 1024.00    | 1009.79    | 25.41 | 0.010            | 20.94            | $T_{\rm L}$                |
| 320-1100 Eq Baseline        | 46  | -13.7002           | -11.9554 | 1034.69    | 1009.22    | 24.17 | 0.010            | 20.96            | T <sub>L</sub> , low η     |
| 320-1100 Eq Baseline        | 47  | -13.6998           | -11.9313 | 1045.18    | 1008.56    | 22.95 | 0.010            | 20.98            | $T_L$ , low $\eta$         |
| 320-1100 Eq Baseline        | 48  | -13.6994           | -11.9073 | 1055.49    | 1007.85    | 21.75 | 0.011            | 21.01            | $T_L$ , low $\eta$         |
| 320-1100 Eq Baseline        | 49  | -13.6990           | -11.8832 | 1065.61    | 1007.08    | 20.58 | 0.011            | 21.03            | $T_L$ , low $\eta$         |
| 320-1100 Eq Baseline        | 50  | -13.6986           | -11.8592 | 1075.56    | 1006.26    | 19.42 | 0.011            | 21.05            | $T_L$ , low $\eta$         |
| 320-1100 Eq Baseline        | 51  | -13.6982           | -11.8352 | 1085.33    | 1005.41    | 18.30 | 0.011            | 21.07            | $T_L$ , low $\eta$         |
| 320-1100 Eq Baseline        | 52  | -13.6977           | -11.8111 | 1094.93    | 1004.52    | 17.20 | 0.011            | 21.09            | $T_L$ , low $\eta$         |

| Category                   | WL<br>(%) | B ∆Gp<br>MAR | B ΔGp<br>Value | T <sub>L</sub> Pred (°C) | T <sub>L</sub><br>MAR(°C) | Visc<br>Pred<br>(P) | TiO <sub>2</sub> wt% | R <sub>2</sub> O<br>wt% | MAR<br>Status          |
|----------------------------|-----------|--------------|----------------|--------------------------|---------------------------|---------------------|----------------------|-------------------------|------------------------|
| 320-1100 Eq Baseline       | 53        | -13.6973     | -11.7871       | 1104.36                  | 1003.60                   | 16.12               | 0.012                | 21.11                   | T <sub>L</sub> , low η |
| 320-1100 Eq Baseline       | 54        | -13.6969     | -11.7630       | 1113.64                  | 1002.66                   | 15.08               | 0.012                | 21.13                   | $T_L$ , low $\eta$     |
| 320-1100 Eq Baseline       | 55        | -13.6965     | -11.7390       | 1122.75                  | 1001.70                   | 14.06               | 0.012                | 21.15                   | $T_L$ , low $\eta$     |
| 320-1100 Eq Baseline       | 56        | -13.6960     | -11.7149       | 1131.71                  | 1000.72                   | 13.07               | 0.012                | 21.17                   | $T_L$ , low $\eta$     |
| 320-1100 Eq Baseline       | 57        | -13.6956     | -11.6909       | 1140.53                  | 999.73                    | 12.12               | 0.013                | 21.19                   | $T_L$ , low $\eta$     |
| 320-1100 Eq Baseline       | 58        | -13.6951     | -11.6669       | 1149.19                  | 998.73                    | 11.20               | 0.013                | 21.22                   | $T_L$ , low $\eta$     |
| 320-1100 Eq Baseline       | 59        | -13.6947     | -11.6428       | 1157.72                  | 997.72                    | 10.31               | 0.013                | 21.24                   | $T_L$ , low $\eta$     |
| 320-1100 Eq Baseline       | 60        | -13.6942     | -11.6188       | 1166.10                  | 996.70                    | 9.46                | 0.013                | 21.26                   | $T_L$ , low $\eta$     |
| 320-1100 Eq Baseline w CST | 25        | -13.7101     | -12.3599       | 748.83                   | 995.96                    | 53.93               | 0.425                | 20.43                   | -                      |
| 320-1100 Eq Baseline w CST | 26        | -13.7099     | -12.3318       | 764.72                   | 998.21                    | 52.51               | 0.442                | 20.45                   | -                      |
| 320-1100 Eq Baseline w CST | 27        | -13.7098     | -12.3038       | 780.25                   | 1000.34                   | 51.09               | 0.459                | 20.46                   | -                      |
| 320-1100 Eq Baseline w CST | 28        | -13.7096     | -12.2757       | 795.43                   | 1002.35                   | 49.68               | 0.476                | 20.48                   | -                      |
| 320-1100 Eq Baseline w CST | 29        | -13.7094     | -12.2477       | 810.26                   | 1003.72                   | 48.27               | 0.493                | 20.50                   | -                      |
| 320-1100 Eq Baseline w CST | 30        | -13.7092     | -12.2196       | 824.77                   | 1004.75                   | 46.86               | 0.510                | 20.51                   | -                      |
| 320-1100 Eq Baseline w CST | 31        | -13.7090     | -12.1915       | 838.97                   | 1005.74                   | 45.46               | 0.527                | 20.53                   | -                      |
| 320-1100 Eq Baseline w CST | 32        | -13.7088     | -12.1635       | 852.86                   | 1006.69                   | 44.06               | 0.544                | 20.55                   | -                      |
| 320-1100 Eq Baseline w CST | 33        | -13.7086     | -12.1354       | 866.46                   | 1007.60                   | 42.67               | 0.561                | 20.56                   | -                      |
| 320-1100 Eq Baseline w CST | 34        | -13.7083     | -12.1074       | 879.77                   | 1008.44                   | 41.28               | 0.578                | 20.58                   | -                      |
| 320-1100 Eq Baseline w CST | 35        | -13.7081     | -12.0793       | 892.82                   | 1009.21                   | 39.91               | 0.595                | 20.60                   | -                      |
| 320-1100 Eq Baseline w CST | 36        | -13.7079     | -12.0513       | 905.60                   | 1009.91                   | 38.54               | 0.612                | 20.62                   | -                      |
| 320-1100 Eq Baseline w CST | 37        | -13.7076     | -12.0232       | 918.12                   | 1010.52                   | 37.18               | 0.629                | 20.63                   | -                      |
| 320-1100 Eq Baseline w CST | 38        | -13.7074     | -11.9951       | 930.40                   | 1011.03                   | 35.83               | 0.646                | 20.65                   | -                      |
| 320-1100 Eq Baseline w CST | 39        | -13.7072     | -11.9671       | 942.43                   | 1011.43                   | 34.49               | 0.663                | 20.67                   | -                      |
| 320-1100 Eq Baseline w CST | 40        | -13.7069     | -11.9390       | 954.23                   | 1011.72                   | 33.16               | 0.680                | 20.68                   | -                      |
| 320-1100 Eq Baseline w CST | 41        | -13.7066     | -11.9110       | 965.81                   | 1011.88                   | 31.85               | 0.697                | 20.70                   | -                      |
| 320-1100 Eq Baseline w CST | 42        | -13.7064     | -11.8829       | 977.16                   | 1011.92                   | 30.54               | 0.714                | 20.72                   | -                      |
| 320-1100 Eq Baseline w CST | 43        | -13.7061     | -11.8549       | 988.30                   | 1011.84                   | 29.25               | 0.731                | 20.74                   | -                      |
| 320-1100 Eq Baseline w CST | 44        | -13.7058     | -11.8268       | 999.24                   | 1011.65                   | 27.98               | 0.748                | 20.75                   | -                      |
| 320-1100 Eq Baseline w CST | 45        | -13.7056     | -11.7987       | 1009.97                  | 1011.35                   | 26.72               | 0.765                | 20.77                   | -                      |
| 320-1100 Eq Baseline w CST | 46        | -13.7053     | -11.7707       | 1020.50                  | 1010.95                   | 25.48               | 0.782                | 20.79                   | $T_{\rm L}$            |
| 320-1100 Eq Baseline w CST | 47        | -13.7050     | -11.7426       | 1030.85                  | 1010.46                   | 24.26               | 0.799                | 20.80                   | $T_L$ , low $\eta$     |
| 320-1100 Eq Baseline w CST | 48        | -13.7047     | -11.7146       | 1041.00                  | 1009.89                   | 23.06               | 0.816                | 20.82                   | $T_L$ , low $\eta$     |

| Category                   | WL  | B \( \Delta G p \) | B \( \Delta G p \) | $T_{\rm L}$ | $T_{\rm L}$ | Visc  | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                    |
|----------------------------|-----|--------------------|--------------------|-------------|-------------|-------|------------------|------------------|------------------------|
|                            | (%) | MAR                | Value              | Pred        | MAR(°C)     | Pred  | wt%              | wt%              | Status                 |
| 220 1100 F. D. L. GGT      | 40  | 12.7044            | 11.6065            | (°C)        | 1000.26     | (P)   | 0.022            | 20.04            |                        |
| 320-1100 Eq Baseline w CST | 49  | -13.7044           | -11.6865           | 1050.98     | 1009.26     | 21.87 | 0.833            | 20.84            | $T_L$ , low $\eta$     |
| 320-1100 Eq Baseline w CST | 50  | -13.7041           | -11.6585           | 1060.78     | 1008.57     | 20.71 | 0.850            | 20.86            | $T_L$ , low $\eta$     |
| 320-1100 Eq Baseline w CST | 51  | -13.7038           | -11.6304           | 1070.40     | 1007.84     | 19.57 | 0.866            | 20.87            | $T_L$ , low $\eta$     |
| 320-1100 Eq Baseline w CST | 52  | -13.7034           | -11.6023           | 1079.86     | 1007.06     | 18.46 | 0.883            | 20.89            | $T_L$ , low $\eta$     |
| 320-1100 Eq Baseline w CST | 53  | -13.7031           | -11.5743           | 1089.16     | 1006.24     | 17.36 | 0.900            | 20.91            | $T_L$ , low $\eta$     |
| 320-1100 Eq Baseline w CST | 54  | -13.7028           | -11.5462           | 1098.29     | 1005.40     | 16.30 | 0.917            | 20.92            | $T_L$ , low $\eta$     |
| 320-1100 Eq Baseline w CST | 55  | -13.7025           | -11.5182           | 1107.27     | 1004.53     | 15.26 | 0.934            | 20.94            | T <sub>L</sub> , low η |
| 320-1100 Eq Baseline w CST | 56  | -13.7021           | -11.4901           | 1116.10     | 1003.64     | 14.25 | 0.951            | 20.96            | T <sub>L</sub> , low η |
| 320-1100 Eq Baseline w CST | 57  | -13.7018           | -11.4621           | 1124.78     | 1002.73     | 13.27 | 0.968            | 20.98            | T <sub>L</sub> , low η |
| 320-1100 Eq Baseline w CST | 58  | -13.7014           | -11.4340           | 1133.31     | 1001.80     | 12.32 | 0.985            | 20.99            | $T_L$ , low $\eta$     |
| 320-1100 Eq Baseline w CST | 59  | -13.7011           | -11.4060           | 1141.71     | 1000.87     | 11.40 | 1.002            | 21.01            | $T_L$ , low $\eta$     |
| 320-1100 Eq Baseline w CST | 60  | -13.7007           | -11.3779           | 1149.96     | 999.92      | 10.51 | 1.019            | 21.03            | T <sub>L</sub> , low η |
| 418-1100 Eq Baseline       | 25  | -13.7200           | -9.6883            | 806.71      | 1000.72     | 91.07 | 0.006            | 17.52            | -                      |
| 418-1100 Eq Baseline       | 26  | -13.7200           | -9.7012            | 822.76      | 1002.86     | 88.67 | 0.006            | 17.58            | -                      |
| 418-1100 Eq Baseline       | 27  | -13.7200           | -9.7141            | 838.39      | 1004.84     | 86.28 | 0.006            | 17.65            | -                      |
| 418-1100 Eq Baseline       | 28  | -13.7200           | -9.7270            | 853.61      | 1006.35     | 83.89 | 0.006            | 17.71            | -                      |
| 418-1100 Eq Baseline       | 29  | -13.7200           | -9.7400            | 868.44      | 1007.27     | 81.50 | 0.006            | 17.77            | -                      |
| 418-1100 Eq Baseline       | 30  | -13.7200           | -9.7529            | 882.90      | 1008.11     | 79.12 | 0.007            | 17.83            | -                      |
| 418-1100 Eq Baseline       | 31  | -13.7200           | -9.7658            | 897.00      | 1008.86     | 76.74 | 0.007            | 17.89            | -                      |
| 418-1100 Eq Baseline       | 32  | -13.7200           | -9.7787            | 910.75      | 1009.51     | 74.38 | 0.007            | 17.95            | -                      |
| 418-1100 Eq Baseline       | 33  | -13.7200           | -9.7916            | 924.17      | 1010.03     | 72.02 | 0.007            | 18.01            | -                      |
| 418-1100 Eq Baseline       | 34  | -13.7200           | -9.8045            | 937.28      | 1010.43     | 69.67 | 0.007            | 18.07            | -                      |
| 418-1100 Eq Baseline       | 35  | -13.7200           | -9.8175            | 950.07      | 1010.70     | 67.34 | 0.008            | 18.13            | -                      |
| 418-1100 Eq Baseline       | 36  | -13.7200           | -9.8304            | 962.57      | 1010.83     | 65.02 | 0.008            | 18.19            | -                      |
| 418-1100 Eq Baseline       | 37  | -13.7200           | -9.8433            | 974.78      | 1010.82     | 62.71 | 0.008            | 18.26            | -                      |
| 418-1100 Eq Baseline       | 38  | -13.7200           | -9.8562            | 986.72      | 1010.68     | 60.42 | 0.008            | 18.32            | -                      |
| 418-1100 Eq Baseline       | 39  | -13.7200           | -9.8691            | 998.39      | 1010.42     | 58.14 | 0.009            | 18.38            | -                      |
| 418-1100 Eq Baseline       | 40  | -13.7200           | -9.8821            | 1009.81     | 1010.04     | 55.89 | 0.009            | 18.44            | -                      |
| 418-1100 Eq Baseline       | 41  | -13.7200           | -9.8950            | 1020.97     | 1009.57     | 53.65 | 0.009            | 18.50            | $T_{ m L}$             |
| 418-1100 Eq Baseline       | 42  | -13.7200           | -9.9079            | 1031.89     | 1009.01     | 51.43 | 0.009            | 18.56            | $T_{ m L}$             |
| 418-1100 Eq Baseline       | 43  | -13.7200           | -9.9208            | 1042.58     | 1008.37     | 49.24 | 0.009            | 18.62            | $T_{ m L}$             |
| 418-1100 Eq Baseline       | 44  | -13.7200           | -9.9337            | 1053.04     | 1007.67     | 47.08 | 0.010            | 18.68            | $T_{ m L}$             |

| Category                   | WL  | BΔGp     | BΔGp     | $T_{\rm L}$  | T <sub>L</sub> | Visc        | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                    |
|----------------------------|-----|----------|----------|--------------|----------------|-------------|------------------|------------------|------------------------|
|                            | (%) | MAR      | Value    | Pred<br>(°C) | MAR(°C)        | Pred<br>(P) | wt%              | wt%              | Status                 |
| 418-1100 Eq Baseline       | 45  | -13.7200 | -9.9466  | 1063.29      | 1006.91        | 44.94       | 0.010            | 18.74            | $T_{ m L}$             |
| 418-1100 Eq Baseline       | 46  | -13.7200 | -9.9596  | 1073.32      | 1006.11        | 42.82       | 0.010            | 18.80            | $T_{ m L}$             |
| 418-1100 Eq Baseline       | 47  | -13.7200 | -9.9725  | 1083.15      | 1005.27        | 40.74       | 0.010            | 18.86            | $T_{ m L}$             |
| 418-1100 Eq Baseline       | 48  | -13.7200 | -9.9854  | 1092.77      | 1004.39        | 38.69       | 0.011            | 18.93            | $T_{ m L}$             |
| 418-1100 Eq Baseline       | 49  | -13.7200 | -9.9983  | 1102.21      | 1003.50        | 36.68       | 0.011            | 18.99            | $T_{ m L}$             |
| 418-1100 Eq Baseline       | 50  | -13.7200 | -10.0112 | 1111.45      | 1002.58        | 34.70       | 0.011            | 19.05            | $T_{ m L}$             |
| 418-1100 Eq Baseline       | 51  | -13.7200 | -10.0241 | 1120.52      | 1001.64        | 32.76       | 0.011            | 19.11            | $T_{ m L}$             |
| 418-1100 Eq Baseline       | 52  | -13.7200 | -10.0371 | 1129.40      | 1000.69        | 30.85       | 0.011            | 19.17            | $T_{ m L}$             |
| 418-1100 Eq Baseline       | 53  | -13.7200 | -10.0500 | 1138.12      | 999.73         | 28.99       | 0.012            | 19.23            | $T_{ m L}$             |
| 418-1100 Eq Baseline       | 54  | -13.7200 | -10.0629 | 1146.66      | 998.76         | 27.18       | 0.012            | 19.29            | $T_{ m L}$             |
| 418-1100 Eq Baseline       | 55  | -13.7200 | -10.0758 | 1155.05      | 997.78         | 25.41       | 0.012            | 19.35            | $T_{ m L}$             |
| 418-1100 Eq Baseline       | 56  | -13.7200 | -10.0887 | 1163.27      | 996.80         | 23.69       | 0.012            | 19.41            | T <sub>L</sub> , low η |
| 418-1100 Eq Baseline       | 57  | -13.7200 | -10.1016 | 1171.34      | 995.81         | 22.02       | 0.013            | 19.47            | T <sub>L</sub> , low η |
| 418-1100 Eq Baseline       | 58  | -13.7200 | -10.1146 | 1179.27      | 994.82         | 20.40       | 0.013            | 19.54            | $T_L$ , low $\eta$     |
| 418-1100 Eq Baseline       | 59  | -13.7200 | -10.1275 | 1187.04      | 993.83         | 18.84       | 0.013            | 19.60            | $T_L$ , low $\eta$     |
| 418-1100 Eq Baseline       | 60  | -13.7200 | -10.1404 | 1194.68      | 992.85         | 17.33       | 0.013            | 19.66            | T <sub>L</sub> , low η |
| 418-1100 Eq Baseline w CST | 25  | -13.7200 | -9.5879  | 796.07       | 999.32         | 92.49       | 0.425            | 17.43            | -                      |
| 418-1100 Eq Baseline w CST | 26  | -13.7200 | -9.5968  | 811.89       | 1001.49        | 90.13       | 0.442            | 17.49            | -                      |
| 418-1100 Eq Baseline w CST | 27  | -13.7200 | -9.6057  | 827.29       | 1003.52        | 87.78       | 0.459            | 17.54            | -                      |
| 418-1100 Eq Baseline w CST | 28  | -13.7200 | -9.6146  | 842.29       | 1005.42        | 85.43       | 0.476            | 17.60            | -                      |
| 418-1100 Eq Baseline w CST | 29  | -13.7200 | -9.6235  | 856.91       | 1006.97        | 83.09       | 0.493            | 17.66            | -                      |
| 418-1100 Eq Baseline w CST | 30  | -13.7200 | -9.6324  | 871.16       | 1007.87        | 80.74       | 0.510            | 17.71            | -                      |
| 418-1100 Eq Baseline w CST | 31  | -13.7200 | -9.6413  | 885.05       | 1008.70        | 78.41       | 0.527            | 17.77            | -                      |
| 418-1100 Eq Baseline w CST | 32  | -13.7200 | -9.6502  | 898.60       | 1009.44        | 76.08       | 0.544            | 17.83            | -                      |
| 418-1100 Eq Baseline w CST | 33  | -13.7200 | -9.6591  | 911.83       | 1010.09        | 73.76       | 0.561            | 17.88            | -                      |
| 418-1100 Eq Baseline w CST | 34  | -13.7200 | -9.6680  | 924.74       | 1010.64        | 71.44       | 0.578            | 17.94            | -                      |
| 418-1100 Eq Baseline w CST | 35  | -13.7200 | -9.6770  | 937.35       | 1011.07        | 69.14       | 0.595            | 18.00            | -                      |
| 418-1100 Eq Baseline w CST | 36  | -13.7200 | -9.6859  | 949.67       | 1011.38        | 66.85       | 0.612            | 18.06            | -                      |
| 418-1100 Eq Baseline w CST | 37  | -13.7200 | -9.6948  | 961.70       | 1011.57        | 64.56       | 0.629            | 18.11            | -                      |
| 418-1100 Eq Baseline w CST | 38  | -13.7200 | -9.7037  | 973.47       | 1011.63        | 62.30       | 0.646            | 18.17            | -                      |
| 418-1100 Eq Baseline w CST | 39  | -13.7200 | -9.7126  | 984.96       | 1011.56        | 60.04       | 0.663            | 18.23            | -                      |
| 418-1100 Eq Baseline w CST | 40  | -13.7200 | -9.7215  | 996.21       | 1011.38        | 57.81       | 0.680            | 18.28            | -                      |

| Category                   | WL  | B ∆Gp    | B ∆Gp    | $T_{\rm L}$ | $T_{ m L}$ | Visc       | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                    |
|----------------------------|-----|----------|----------|-------------|------------|------------|------------------|------------------|------------------------|
|                            | (%) | MAR      | Value    | Pred        | MAR(°C)    | Pred       | wt%              | wt%              | Status                 |
|                            |     |          |          | (°C)        |            | <b>(P)</b> |                  |                  |                        |
| 418-1100 Eq Baseline w CST | 41  | -13.7200 | -9.7304  | 1007.21     | 1011.09    | 55.59      | 0.697            | 18.34            | -                      |
| 418-1100 Eq Baseline w CST | 42  | -13.7200 | -9.7393  | 1017.97     | 1010.70    | 53.39      | 0.714            | 18.40            | $T_{ m L}$             |
| 418-1100 Eq Baseline w CST | 43  | -13.7200 | -9.7482  | 1028.50     | 1010.22    | 51.20      | 0.731            | 18.46            | $T_{ m L}$             |
| 418-1100 Eq Baseline w CST | 44  | -13.7200 | -9.7571  | 1038.80     | 1009.67    | 49.05      | 0.748            | 18.51            | $T_{ m L}$             |
| 418-1100 Eq Baseline w CST | 45  | -13.7200 | -9.7660  | 1048.90     | 1009.05    | 46.91      | 0.765            | 18.57            | $T_{ m L}$             |
| 418-1100 Eq Baseline w CST | 46  | -13.7200 | -9.7749  | 1058.78     | 1008.37    | 44.80      | 0.782            | 18.63            | $T_{ m L}$             |
| 418-1100 Eq Baseline w CST | 47  | -13.7200 | -9.7838  | 1068.45     | 1007.65    | 42.72      | 0.799            | 18.68            | $T_{ m L}$             |
| 418-1100 Eq Baseline w CST | 48  | -13.7200 | -9.7927  | 1077.93     | 1006.89    | 40.67      | 0.816            | 18.74            | $T_{ m L}$             |
| 418-1100 Eq Baseline w CST | 49  | -13.7200 | -9.8016  | 1087.22     | 1006.09    | 38.64      | 0.833            | 18.80            | $T_{ m L}$             |
| 418-1100 Eq Baseline w CST | 50  | -13.7200 | -9.8105  | 1096.33     | 1005.27    | 36.65      | 0.850            | 18.86            | $T_{ m L}$             |
| 418-1100 Eq Baseline w CST | 51  | -13.7200 | -9.8194  | 1105.25     | 1004.42    | 34.70      | 0.866            | 18.91            | $T_{ m L}$             |
| 418-1100 Eq Baseline w CST | 52  | -13.7200 | -9.8283  | 1114.00     | 1003.56    | 32.78      | 0.883            | 18.97            | $T_{ m L}$             |
| 418-1100 Eq Baseline w CST | 53  | -13.7200 | -9.8372  | 1122.58     | 1002.67    | 30.90      | 0.900            | 19.03            | $T_{ m L}$             |
| 418-1100 Eq Baseline w CST | 54  | -13.7200 | -9.8461  | 1130.99     | 1001.78    | 29.06      | 0.917            | 19.08            | $T_{ m L}$             |
| 418-1100 Eq Baseline w CST | 55  | -13.7200 | -9.8550  | 1139.24     | 1000.88    | 27.26      | 0.934            | 19.14            | $T_{ m L}$             |
| 418-1100 Eq Baseline w CST | 56  | -13.7200 | -9.8639  | 1147.34     | 999.97     | 25.51      | 0.951            | 19.20            | $T_{ m L}$             |
| 418-1100 Eq Baseline w CST | 57  | -13.7200 | -9.8728  | 1155.28     | 999.05     | 23.80      | 0.968            | 19.26            | $T_L$ , low $\eta$     |
| 418-1100 Eq Baseline w CST | 58  | -13.7200 | -9.8817  | 1163.08     | 998.13     | 22.15      | 0.985            | 19.31            | T <sub>L</sub> , low η |
| 418-1100 Eq Baseline w CST | 59  | -13.7200 | -9.8906  | 1170.73     | 997.20     | 20.54      | 1.002            | 19.37            | T <sub>L</sub> , low η |
| 418-1100 Eq Baseline w CST | 60  | -13.7200 | -9.8995  | 1178.24     | 996.28     | 18.99      | 1.019            | 19.43            | T <sub>L</sub> , low η |
| 440-1100 Eq Baseline       | 25  | -13.5929 | -14.6852 | 727.09      | 993.57     | 58.92      | 0.006            | 22.77            | $\Delta G_{ m P}$      |
| 440-1100 Eq Baseline       | 26  | -13.5942 | -14.6315 | 743.00      | 995.80     | 57.24      | 0.006            | 22.76            | $\Delta G_{ m P}$      |
| 440-1100 Eq Baseline       | 27  | -13.5955 | -14.5778 | 758.57      | 997.70     | 55.57      | 0.006            | 22.76            | $\Delta G_{ m P}$      |
| 440-1100 Eq Baseline       | 28  | -13.5968 | -14.5241 | 773.82      | 998.77     | 53.90      | 0.006            | 22.75            | $\Delta G_{ m P}$      |
| 440-1100 Eq Baseline       | 29  | -13.5981 | -14.4704 | 788.76      | 999.82     | 52.24      | 0.006            | 22.74            | $\Delta G_{ m P}$      |
| 440-1100 Eq Baseline       | 30  | -13.5994 | -14.4166 | 803.40      | 1000.85    | 50.59      | 0.007            | 22.73            | $\Delta G_{ m P}$      |
| 440-1100 Eq Baseline       | 31  | -13.6006 | -14.3629 | 817.75      | 1001.85    | 48.95      | 0.007            | 22.72            | $\Delta G_{ m P}$      |
| 440-1100 Eq Baseline       | 32  | -13.6019 | -14.3092 | 831.83      | 1002.83    | 47.32      | 0.007            | 22.71            | $\Delta G_{ m P}$      |
| 440-1100 Eq Baseline       | 33  | -13.6032 | -14.2555 | 845.64      | 1003.78    | 45.70      | 0.007            | 22.70            | $\Delta G_{ m P}$      |
| 440-1100 Eq Baseline       | 34  | -13.6044 | -14.2018 | 859.19      | 1004.68    | 44.09      | 0.007            | 22.69            | $\Delta G_{ m P}$      |
| 440-1100 Eq Baseline       | 35  | -13.6057 | -14.1481 | 872.49      | 1005.53    | 42.49      | 0.008            | 22.68            | $\Delta G_{ m P}$      |
| 440-1100 Eq Baseline       | 36  | -13.6069 | -14.0944 | 885.55      | 1006.32    | 40.91      | 0.008            | 22.67            | $\Delta G_{ m P}$      |

| Category                   | WL<br>(%) | B ΔGp<br>MAR | B ΔGp<br>Value | T <sub>L</sub><br>Pred<br>(°C) | T <sub>L</sub><br>MAR(°C) | Visc<br>Pred<br>(P) | TiO <sub>2</sub> wt% | R <sub>2</sub> O<br>wt% | MAR<br>Status                 |
|----------------------------|-----------|--------------|----------------|--------------------------------|---------------------------|---------------------|----------------------|-------------------------|-------------------------------|
| 440-1100 Eq Baseline       | 37        | -13.6081     | -14.0407       | 898.37                         | 1007.05                   | 39.34               | 0.008                | 22.67                   | $\Delta G_{ m P}$             |
| 440-1100 Eq Baseline       | 38        | -13.6094     | -13.9870       | 910.97                         | 1007.70                   | 37.79               | 0.008                | 22.66                   | $\Delta G_{P}$                |
| 440-1100 Eq Baseline       | 39        | -13.6106     | -13.9333       | 923.34                         | 1008.27                   | 36.25               | 0.009                | 22.65                   | $\Delta G_{P}$                |
| 440-1100 Eq Baseline       | 40        | -13.6118     | -13.8796       | 935.51                         | 1008.75                   | 34.73               | 0.009                | 22.64                   | $\Delta G_{P}$                |
| 440-1100 Eq Baseline       | 41        | -13.6130     | -13.8259       | 947.46                         | 1009.12                   | 33.23               | 0.009                | 22.63                   | $\Delta G_{ m P}$             |
| 440-1100 Eq Baseline       | 42        | -13.6142     | -13.7722       | 959.22                         | 1009.38                   | 31.75               | 0.009                | 22.62                   | $\Delta G_{P}$                |
| 440-1100 Eq Baseline       | 43        | -13.6154     | -13.7184       | 970.77                         | 1009.54                   | 30.29               | 0.009                | 22.61                   | $\Delta G_{ m P}$             |
| 440-1100 Eq Baseline       | 44        | -13.6166     | -13.6647       | 982.14                         | 1009.57                   | 28.85               | 0.010                | 22.60                   | $\Delta G_{P}$                |
| 440-1100 Eq Baseline       | 45        | -13.6178     | -13.6110       | 993.32                         | 1009.50                   | 27.44               | 0.010                | 22.59                   | $\Delta G_{P}$                |
| 440-1100 Eq Baseline       | 46        | -13.6190     | -13.5573       | 1004.32                        | 1009.31                   | 26.05               | 0.010                | 22.58                   | $\Delta G_{P}$                |
| 440-1100 Eq Baseline       | 47        | -13.6202     | -13.5036       | 1015.14                        | 1009.02                   | 24.69               | 0.010                | 22.57                   | $\Delta G_P$ , $T_L$ , low    |
|                            |           |              |                |                                |                           |                     |                      |                         | $\eta$ $\Delta G_P, T_L, low$ |
| 440-1100 Eq Baseline       | 48        | -13.6213     | -13.4499       | 1025.79                        | 1008.64                   | 23.35               | 0.011                | 22.57                   | $\Delta G_P$ , $T_L$ , low    |
|                            |           |              |                |                                |                           |                     |                      |                         | η                             |
| 440-1100 Eq Baseline       | 49        | -13.6225     | -13.3962       | 1036.27                        | 1008.16                   | 22.04               | 0.011                | 22.56                   | $\Delta G_P$ , $T_L$ , low    |
|                            |           |              |                |                                |                           |                     |                      |                         | η                             |
| 440-1100 Eq Baseline       | 50        | -13.6237     | -13.3425       | 1046.59                        | 1007.61                   | 20.76               | 0.011                | 22.55                   | $T_L$ , low $\eta$            |
| 440-1100 Eq Baseline       | 51        | -13.6248     | -13.2888       | 1056.75                        | 1006.98                   | 19.51               | 0.011                | 22.54                   | $T_L$ , low $\eta$            |
| 440-1100 Eq Baseline       | 52        | -13.6259     | -13.2351       | 1066.76                        | 1006.30                   | 18.29               | 0.011                | 22.53                   | $T_L$ , low $\eta$            |
| 440-1100 Eq Baseline       | 53        | -13.6271     | -13.1814       | 1076.61                        | 1005.56                   | 17.10               | 0.012                | 22.52                   | $T_L$ , low $\eta$            |
| 440-1100 Eq Baseline       | 54        | -13.6282     | -13.1277       | 1086.31                        | 1004.77                   | 15.95               | 0.012                | 22.51                   | $T_L$ , low $\eta$            |
| 440-1100 Eq Baseline       | 55        | -13.6293     | -13.0739       | 1095.87                        | 1003.94                   | 14.84               | 0.012                | 22.50                   | $T_L$ , low $\eta$            |
| 440-1100 Eq Baseline       | 56        | -13.6304     | -13.0202       | 1105.29                        | 1003.08                   | 13.76               | 0.012                | 22.49                   | $T_L$ , low $\eta$            |
| 440-1100 Eq Baseline       | 57        | -13.6316     | -12.9665       | 1114.57                        | 1002.18                   | 12.72               | 0.013                | 22.48                   | $T_L$ , low $\eta$            |
| 440-1100 Eq Baseline       | 58        | -13.6327     | -12.9128       | 1123.71                        | 1001.26                   | 11.72               | 0.013                | 22.48                   | $T_L$ , low $\eta$            |
| 440-1100 Eq Baseline       | 59        | -13.6337     | -12.8591       | 1132.73                        | 1000.31                   | 10.75               | 0.013                | 22.47                   | $T_L$ , low $\eta$            |
| 440-1100 Eq Baseline       | 60        | -13.6348     | -12.8054       | 1141.61                        | 999.35                    | 9.83                | 0.013                | 22.46                   | $T_L$ , low $\eta$            |
| 440-1100 Eq Baseline w CST | 25        | -13.5955     | -14.5848       | 717.04                         | 992.02                    | 60.03               | 0.425                | 22.68                   | $\Delta G_{ m P}$             |
| 440-1100 Eq Baseline w CST | 26        | -13.5969     | -14.5271       | 732.70                         | 994.25                    | 58.38               | 0.442                | 22.67                   | $\Delta G_{P}$                |
| 440-1100 Eq Baseline w CST | 27        | -13.5983     | -14.4694       | 748.04                         | 996.36                    | 56.74               | 0.459                | 22.65                   | $\Delta G_{P}$                |
| 440-1100 Eq Baseline w CST | 28        | -13.5996     | -14.4117       | 763.06                         | 998.19                    | 55.10               | 0.476                | 22.64                   | $\Delta G_{P}$                |
| 440-1100 Eq Baseline w CST | 29        | -13.6010     | -14.3539       | 777.77                         | 999.21                    | 53.47               | 0.493                | 22.63                   | $\Delta G_{P}$                |

| Category                   | WL  | B ∆Gp    | B \( \Delta G p \) | $T_{ m L}$ | $T_{ m L}$ | Visc       | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                    |
|----------------------------|-----|----------|--------------------|------------|------------|------------|------------------|------------------|------------------------|
|                            | (%) | MAR      | Value              | Pred       | MAR(°C)    | Pred       | wt%              | wt%              | Status                 |
|                            | , , |          |                    | (°C)       |            | <b>(P)</b> |                  |                  |                        |
| 440-1100 Eq Baseline w CST | 30  | -13.6024 | -14.2962           | 792.19     | 1000.21    | 51.85      | 0.510            | 22.61            | $\Delta G_{P}$         |
| 440-1100 Eq Baseline w CST | 31  | -13.6038 | -14.2385           | 806.33     | 1001.20    | 50.23      | 0.527            | 22.60            | $\Delta G_{P}$         |
| 440-1100 Eq Baseline w CST | 32  | -13.6052 | -14.1808           | 820.20     | 1002.16    | 48.62      | 0.544            | 22.59            | $\Delta G_{P}$         |
| 440-1100 Eq Baseline w CST | 33  | -13.6065 | -14.1230           | 833.80     | 1003.10    | 47.02      | 0.561            | 22.57            | $\Delta G_{P}$         |
| 440-1100 Eq Baseline w CST | 34  | -13.6079 | -14.0653           | 847.15     | 1004.00    | 45.44      | 0.578            | 22.56            | $\Delta G_{P}$         |
| 440-1100 Eq Baseline w CST | 35  | -13.6092 | -14.0076           | 860.25     | 1004.86    | 43.86      | 0.595            | 22.55            | $\Delta G_{P}$         |
| 440-1100 Eq Baseline w CST | 36  | -13.6106 | -13.9499           | 873.11     | 1005.68    | 42.30      | 0.612            | 22.54            | $\Delta G_{P}$         |
| 440-1100 Eq Baseline w CST | 37  | -13.6119 | -13.8921           | 885.75     | 1006.45    | 40.74      | 0.629            | 22.52            | $\Delta G_{P}$         |
| 440-1100 Eq Baseline w CST | 38  | -13.6133 | -13.8344           | 898.16     | 1007.15    | 39.20      | 0.646            | 22.51            | $\Delta G_{P}$         |
| 440-1100 Eq Baseline w CST | 39  | -13.6146 | -13.7767           | 910.35     | 1007.80    | 37.68      | 0.663            | 22.50            | $\Delta G_{P}$         |
| 440-1100 Eq Baseline w CST | 40  | -13.6159 | -13.7190           | 922.33     | 1008.36    | 36.17      | 0.680            | 22.48            | $\Delta G_{P}$         |
| 440-1100 Eq Baseline w CST | 41  | -13.6172 | -13.6613           | 934.11     | 1008.85    | 34.68      | 0.697            | 22.47            | $\Delta G_{P}$         |
| 440-1100 Eq Baseline w CST | 42  | -13.6185 | -13.6035           | 945.69     | 1009.24    | 33.20      | 0.714            | 22.46            | $\Delta G_{P}$         |
| 440-1100 Eq Baseline w CST | 43  | -13.6198 | -13.5458           | 957.08     | 1009.54    | 31.75      | 0.731            | 22.45            | $\Delta G_{P}$         |
| 440-1100 Eq Baseline w CST | 44  | -13.6211 | -13.4881           | 968.28     | 1009.74    | 30.31      | 0.748            | 22.43            | $\Delta G_{P}$         |
| 440-1100 Eq Baseline w CST | 45  | -13.6224 | -13.4304           | 979.29     | 1009.84    | 28.89      | 0.765            | 22.42            | $\Delta G_{P}$         |
| 440-1100 Eq Baseline w CST | 46  | -13.6237 | -13.3726           | 990.13     | 1009.83    | 27.50      | 0.782            | 22.41            | -                      |
| 440-1100 Eq Baseline w CST | 47  | -13.6250 | -13.3149           | 1000.79    | 1009.73    | 26.13      | 0.799            | 22.39            | -                      |
| 440-1100 Eq Baseline w CST | 48  | -13.6263 | -13.2572           | 1011.29    | 1009.53    | 24.78      | 0.816            | 22.38            | $T_L$ , low $\eta$     |
| 440-1100 Eq Baseline w CST | 49  | -13.6275 | -13.1995           | 1021.61    | 1009.23    | 23.46      | 0.833            | 22.37            | $T_L$ , low $\eta$     |
| 440-1100 Eq Baseline w CST | 50  | -13.6288 | -13.1418           | 1031.78    | 1008.86    | 22.17      | 0.850            | 22.36            | T <sub>L</sub> , low η |
| 440-1100 Eq Baseline w CST | 51  | -13.6301 | -13.0840           | 1041.79    | 1008.40    | 20.90      | 0.866            | 22.34            | T <sub>L</sub> , low η |
| 440-1100 Eq Baseline w CST | 52  | -13.6313 | -13.0263           | 1051.65    | 1007.87    | 19.66      | 0.883            | 22.33            | $T_L$ , low $\eta$     |
| 440-1100 Eq Baseline w CST | 53  | -13.6325 | -12.9686           | 1061.36    | 1007.28    | 18.46      | 0.900            | 22.32            | $T_L$ , low $\eta$     |
| 440-1100 Eq Baseline w CST | 54  | -13.6338 | -12.9109           | 1070.92    | 1006.64    | 17.28      | 0.917            | 22.30            | $T_L$ , low $\eta$     |
| 440-1100 Eq Baseline w CST | 55  | -13.6350 | -12.8531           | 1080.33    | 1005.95    | 16.14      | 0.934            | 22.29            | $T_L$ , low $\eta$     |
| 440-1100 Eq Baseline w CST | 56  | -13.6362 | -12.7954           | 1089.61    | 1005.21    | 15.03      | 0.951            | 22.28            | $T_L$ , low $\eta$     |
| 440-1100 Eq Baseline w CST | 57  | -13.6374 | -12.7377           | 1098.75    | 1004.43    | 13.96      | 0.968            | 22.27            | $T_L$ , low $\eta$     |
| 440-1100 Eq Baseline w CST | 58  | -13.6386 | -12.6800           | 1107.76    | 1003.62    | 12.92      | 0.985            | 22.25            | $T_L$ , low $\eta$     |
| 440-1100 Eq Baseline w CST | 59  | -13.6398 | -12.6223           | 1116.64    | 1002.79    | 11.92      | 1.002            | 22.24            | $T_L$ , low $\eta$     |
| 440-1100 Eq Baseline w CST | 60  | -13.6410 | -12.5645           | 1125.39    | 1001.92    | 10.96      | 1.019            | 22.23            | $T_L$ , low $\eta$     |
| 320-1200 Eq. Baseline      | 25  | -13.7009 | -12.6143           | 755.92     | 997.15     | 53.10      | 0.005            | 20.86            | 1L, 10W I              |
| 320-1200 Eq. Dascille      | 23  | -13.7009 | -12.0143           | 133.72     | 771.13     | 33.10      | 0.003            | 20.00            | _                      |

| Category              | WL<br>(%) | B ΔGp<br>MAR | B ΔGp<br>Value | T <sub>L</sub> Pred | T <sub>L</sub><br>MAR(°C) | Visc<br>Pred | TiO <sub>2</sub> wt% | R <sub>2</sub> O<br>wt% | MAR<br>Status      |
|-----------------------|-----------|--------------|----------------|---------------------|---------------------------|--------------|----------------------|-------------------------|--------------------|
| 320-1200 Eq. Baseline | 26        | -13.7004     | -12.5964       | (°C)<br>771.79      | 999.36                    | (P)<br>51.65 | 0.005                | 20.90                   |                    |
| 320-1200 Eq. Baseline | 27        | -13.7004     | -12.5785       | 787.28              | 1000.60                   | 50.20        | 0.005                | 20.93                   | -                  |
| 320-1200 Eq. Baseline | 28        | -13.6993     | -12.5606       | 802.41              | 1000.65                   | 48.76        | 0.003                | 20.93                   | -                  |
| 320-1200 Eq. Baseline | 29        | -13.6987     | -12.5427       | 817.19              | 1001.05                   | 47.33        | 0.006                | 21.00                   | _                  |
| 320-1200 Eq. Baseline | 30        | -13.6981     | -12.5248       | 831.63              | 1002.60                   | 45.89        | 0.006                | 21.04                   |                    |
| 320-1200 Eq. Baseline | 31        | -13.6976     | -12.5070       | 845.74              | 1003.04                   | 44.47        | 0.006                | 21.07                   | _                  |
| 320-1200 Eq. Baseline | 32        | -13.6970     | -12.4891       | 859.55              | 1005.44                   | 43.05        | 0.006                | 21.11                   | _                  |
| 320-1200 Eq. Baseline | 33        | -13.6964     | -12.4712       | 873.05              | 1006.24                   | 41.64        | 0.007                | 21.14                   | -                  |
| 320-1200 Eq. Baseline | 34        | -13.6958     | -12.4533       | 886.26              | 1006.98                   | 40.23        | 0.007                | 21.18                   | -                  |
| 320-1200 Eq. Baseline | 35        | -13.6952     | -12.4354       | 899.19              | 1007.63                   | 38.84        | 0.007                | 21.21                   | -                  |
| 320-1200 Eq. Baseline | 36        | -13.6946     | -12.4175       | 911.85              | 1008.19                   | 37.45        | 0.007                | 21.24                   | -                  |
| 320-1200 Eq. Baseline | 37        | -13.6940     | -12.3997       | 924.25              | 1008.65                   | 36.08        | 0.007                | 21.28                   | -                  |
| 320-1200 Eq. Baseline | 38        | -13.6934     | -12.3818       | 936.39              | 1009.00                   | 34.71        | 0.008                | 21.31                   | -                  |
| 320-1200 Eq. Baseline | 39        | -13.6928     | -12.3639       | 948.29              | 1009.24                   | 33.36        | 0.008                | 21.35                   | -                  |
| 320-1200 Eq. Baseline | 40        | -13.6922     | -12.3460       | 959.94              | 1009.35                   | 32.02        | 0.008                | 21.38                   | -                  |
| 320-1200 Eq. Baseline | 41        | -13.6915     | -12.3281       | 971.37              | 1009.35                   | 30.69        | 0.008                | 21.42                   | -                  |
| 320-1200 Eq. Baseline | 42        | -13.6909     | -12.3103       | 982.57              | 1009.23                   | 29.38        | 0.008                | 21.45                   | -                  |
| 320-1200 Eq. Baseline | 43        | -13.6902     | -12.2924       | 993.55              | 1009.00                   | 28.09        | 0.009                | 21.49                   | -                  |
| 320-1200 Eq. Baseline | 44        | -13.6896     | -12.2745       | 1004.31             | 1008.67                   | 26.81        | 0.009                | 21.52                   | -                  |
| 320-1200 Eq. Baseline | 45        | -13.6889     | -12.2566       | 1014.88             | 1008.25                   | 25.55        | 0.009                | 21.56                   | $T_{ m L}$         |
| 320-1200 Eq. Baseline | 46        | -13.6883     | -12.2387       | 1025.24             | 1007.75                   | 24.30        | 0.009                | 21.59                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline | 47        | -13.6876     | -12.2208       | 1035.41             | 1007.17                   | 23.08        | 0.009                | 21.63                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline | 48        | -13.6870     | -12.2030       | 1045.38             | 1006.54                   | 21.88        | 0.010                | 21.66                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline | 49        | -13.6863     | -12.1851       | 1055.18             | 1005.84                   | 20.70        | 0.010                | 21.69                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline | 50        | -13.6856     | -12.1672       | 1064.79             | 1005.11                   | 19.55        | 0.010                | 21.73                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline | 51        | -13.6849     | -12.1493       | 1074.23             | 1004.33                   | 18.41        | 0.010                | 21.76                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline | 52        | -13.6842     | -12.1314       | 1083.50             | 1003.51                   | 17.31        | 0.010                | 21.80                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline | 53        | -13.6835     | -12.1136       | 1092.61             | 1002.67                   | 16.23        | 0.011                | 21.83                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline | 54        | -13.6828     | -12.0957       | 1101.55             | 1001.81                   | 15.18        | 0.011                | 21.87                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline | 55        | -13.6821     | -12.0778       | 1110.33             | 1000.92                   | 14.16        | 0.011                | 21.90                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline | 56        | -13.6814     | -12.0599       | 1118.96             | 1000.02                   | 13.17        | 0.011                | 21.94                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline | 57        | -13.6807     | -12.0420       | 1127.45             | 999.10                    | 12.21        | 0.011                | 21.97                   | $T_L$ , low $\eta$ |

| Category                    | WL<br>(%) | B ΔGp<br>MAR | B ∆Gp<br>Value | T <sub>L</sub><br>Pred<br>(°C) | T <sub>L</sub><br>MAR(°C) | Visc<br>Pred<br>(P) | TiO <sub>2</sub> wt% | R <sub>2</sub> O<br>wt% | MAR<br>Status      |
|-----------------------------|-----------|--------------|----------------|--------------------------------|---------------------------|---------------------|----------------------|-------------------------|--------------------|
| 320-1200 Eq. Baseline       | 58        | -13.6800     | -12.0241       | 1135.78                        | 998.18                    | 11.28               | 0.012                | 22.01                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline       | 59        | -13.6793     | -12.0063       | 1143.98                        | 997.24                    | 10.39               | 0.012                | 22.04                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline       | 60        | -13.6785     | -11.9884       | 1152.03                        | 996.29                    | 9.53                | 0.012                | 22.07                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline w CST | 25        | -13.7041     | -12.5070       | 746.14                         | 995.74                    | 54.06               | 0.418                | 20.75                   | -                  |
| 320-1200 Eq. Baseline w CST | 26        | -13.7036     | -12.4849       | 761.80                         | 997.97                    | 52.64               | 0.435                | 20.78                   | -                  |
| 320-1200 Eq. Baseline w CST | 27        | -13.7032     | -12.4627       | 777.09                         | 1000.07                   | 51.22               | 0.452                | 20.81                   | -                  |
| 320-1200 Eq. Baseline w CST | 28        | -13.7028     | -12.4405       | 792.02                         | 1001.33                   | 49.81               | 0.468                | 20.84                   | -                  |
| 320-1200 Eq. Baseline w CST | 29        | -13.7023     | -12.4183       | 806.61                         | 1002.34                   | 48.40               | 0.485                | 20.87                   | -                  |
| 320-1200 Eq. Baseline w CST | 30        | -13.7019     | -12.3962       | 820.86                         | 1003.32                   | 46.99               | 0.502                | 20.90                   | -                  |
| 320-1200 Eq. Baseline w CST | 31        | -13.7014     | -12.3740       | 834.80                         | 1004.27                   | 45.59               | 0.519                | 20.93                   | -                  |
| 320-1200 Eq. Baseline w CST | 32        | -13.7010     | -12.3518       | 848.42                         | 1005.17                   | 44.19               | 0.535                | 20.96                   | -                  |
| 320-1200 Eq. Baseline w CST | 33        | -13.7005     | -12.3297       | 861.75                         | 1006.03                   | 42.80               | 0.552                | 20.99                   | -                  |
| 320-1200 Eq. Baseline w CST | 34        | -13.7000     | -12.3075       | 874.80                         | 1006.82                   | 41.42               | 0.569                | 21.02                   | -                  |
| 320-1200 Eq. Baseline w CST | 35        | -13.6996     | -12.2853       | 887.57                         | 1007.55                   | 40.04               | 0.586                | 21.05                   | -                  |
| 320-1200 Eq. Baseline w CST | 36        | -13.6991     | -12.2632       | 900.07                         | 1008.20                   | 38.67               | 0.602                | 21.08                   | -                  |
| 320-1200 Eq. Baseline w CST | 37        | -13.6986     | -12.2410       | 912.31                         | 1008.77                   | 37.31               | 0.619                | 21.11                   | -                  |
| 320-1200 Eq. Baseline w CST | 38        | -13.6981     | -12.2188       | 924.30                         | 1009.25                   | 35.96               | 0.636                | 21.14                   | -                  |
| 320-1200 Eq. Baseline w CST | 39        | -13.6976     | -12.1966       | 936.05                         | 1009.63                   | 34.62               | 0.652                | 21.17                   | -                  |
| 320-1200 Eq. Baseline w CST | 40        | -13.6971     | -12.1745       | 947.56                         | 1009.90                   | 33.29               | 0.669                | 21.20                   | -                  |
| 320-1200 Eq. Baseline w CST | 41        | -13.6966     | -12.1523       | 958.84                         | 1010.07                   | 31.97               | 0.686                | 21.23                   | -                  |
| 320-1200 Eq. Baseline w CST | 42        | -13.6961     | -12.1301       | 969.90                         | 1010.12                   | 30.67               | 0.703                | 21.26                   | -                  |
| 320-1200 Eq. Baseline w CST | 43        | -13.6955     | -12.1080       | 980.75                         | 1010.07                   | 29.38               | 0.719                | 21.29                   | -                  |
| 320-1200 Eq. Baseline w CST | 44        | -13.6950     | -12.0858       | 991.38                         | 1009.91                   | 28.10               | 0.736                | 21.32                   | -                  |
| 320-1200 Eq. Baseline w CST | 45        | -13.6945     | -12.0636       | 1001.81                        | 1009.65                   | 26.84               | 0.753                | 21.35                   | -                  |
| 320-1200 Eq. Baseline w CST | 46        | -13.6939     | -12.0414       | 1012.05                        | 1009.31                   | 25.60               | 0.770                | 21.38                   | ${ m T_L}$         |
| 320-1200 Eq. Baseline w CST | 47        | -13.6934     | -12.0193       | 1022.09                        | 1008.88                   | 24.37               | 0.786                | 21.41                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline w CST | 48        | -13.6928     | -11.9971       | 1031.94                        | 1008.38                   | 23.17               | 0.803                | 21.44                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline w CST | 49        | -13.6923     | -11.9749       | 1041.61                        | 1007.81                   | 21.98               | 0.820                | 21.47                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline w CST | 50        | -13.6917     | -11.9528       | 1051.11                        | 1007.19                   | 20.81               | 0.837                | 21.50                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline w CST | 51        | -13.6912     | -11.9306       | 1060.43                        | 1006.52                   | 19.67               | 0.853                | 21.53                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline w CST | 52        | -13.6906     | -11.9084       | 1069.58                        | 1005.81                   | 18.55               | 0.870                | 21.56                   | $T_L$ , low $\eta$ |
| 320-1200 Eq. Baseline w CST | 53        | -13.6900     | -11.8862       | 1078.57                        | 1005.06                   | 17.46               | 0.887                | 21.59                   | $T_L$ , low $\eta$ |

| Category                    | WL  | B ∆Gp    | B ∆Gp    | $T_{ m L}$ | $T_{\rm L}$ | Visc  | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                    |
|-----------------------------|-----|----------|----------|------------|-------------|-------|------------------|------------------|------------------------|
|                             | (%) | MAR      | Value    | Pred       | MAR(°C)     | Pred  | wt%              | wt%              | Status                 |
|                             |     |          |          | (°C)       |             | (P)   |                  |                  |                        |
| 320-1200 Eq. Baseline w CST | 54  | -13.6894 | -11.8641 | 1087.40    | 1004.28     | 16.39 | 0.903            | 21.62            | $T_L$ , low $\eta$     |
| 320-1200 Eq. Baseline w CST | 55  | -13.6888 | -11.8419 | 1096.08    | 1003.48     | 15.34 | 0.920            | 21.65            | $T_L$ , low $\eta$     |
| 320-1200 Eq. Baseline w CST | 56  | -13.6882 | -11.8197 | 1104.60    | 1002.66     | 14.33 | 0.937            | 21.68            | $T_L$ , low $\eta$     |
| 320-1200 Eq. Baseline w CST | 57  | -13.6876 | -11.7976 | 1112.97    | 1001.81     | 13.34 | 0.954            | 21.71            | $T_L$ , low $\eta$     |
| 320-1200 Eq. Baseline w CST | 58  | -13.6870 | -11.7754 | 1121.20    | 1000.96     | 12.39 | 0.970            | 21.74            | T <sub>L</sub> , low η |
| 320-1200 Eq. Baseline w CST | 59  | -13.6864 | -11.7532 | 1129.29    | 1000.08     | 11.46 | 0.987            | 21.77            | $T_L$ , low $\eta$     |
| 320-1200 Eq. Baseline w CST | 60  | -13.6858 | -11.7311 | 1137.24    | 999.20      | 10.57 | 1.004            | 21.80            | $T_L$ , low $\eta$     |
| 418-1200 Eq. Baseline       | 25  | -13.7200 | -9.8423  | 802.54     | 1000.32     | 91.33 | 0.005            | 17.86            | -                      |
| 418-1200 Eq. Baseline       | 26  | -13.7200 | -9.8614  | 818.30     | 1002.42     | 88.93 | 0.005            | 17.94            | -                      |
| 418-1200 Eq. Baseline       | 27  | -13.7200 | -9.8804  | 833.63     | 1003.76     | 86.54 | 0.005            | 18.01            | -                      |
| 418-1200 Eq. Baseline       | 28  | -13.7200 | -9.8995  | 848.55     | 1004.71     | 84.15 | 0.006            | 18.09            | -                      |
| 418-1200 Eq. Baseline       | 29  | -13.7200 | -9.9186  | 863.08     | 1005.59     | 81.77 | 0.006            | 18.16            | -                      |
| 418-1200 Eq. Baseline       | 30  | -13.7200 | -9.9377  | 877.22     | 1006.39     | 79.39 | 0.006            | 18.24            | -                      |
| 418-1200 Eq. Baseline       | 31  | -13.7200 | -9.9568  | 891.01     | 1007.10     | 77.02 | 0.006            | 18.31            | -                      |
| 418-1200 Eq. Baseline       | 32  | -13.7200 | -9.9758  | 904.45     | 1007.71     | 74.66 | 0.006            | 18.39            | -                      |
| 418-1200 Eq. Baseline       | 33  | -13.7200 | -9.9949  | 917.55     | 1008.22     | 72.30 | 0.007            | 18.46            | -                      |
| 418-1200 Eq. Baseline       | 34  | -13.7200 | -10.0140 | 930.33     | 1008.61     | 69.96 | 0.007            | 18.54            | -                      |
| 418-1200 Eq. Baseline       | 35  | -13.7200 | -10.0331 | 942.80     | 1008.88     | 67.62 | 0.007            | 18.61            | -                      |
| 418-1200 Eq. Baseline       | 36  | -13.7200 | -10.0521 | 954.98     | 1009.03     | 65.30 | 0.007            | 18.68            | -                      |
| 418-1200 Eq. Baseline       | 37  | -13.7200 | -10.0712 | 966.87     | 1009.05     | 62.99 | 0.007            | 18.76            | -                      |
| 418-1200 Eq. Baseline       | 38  | -13.7200 | -10.0903 | 978.48     | 1008.96     | 60.70 | 0.008            | 18.83            | -                      |
| 418-1200 Eq. Baseline       | 39  | -13.7200 | -10.1094 | 989.82     | 1008.75     | 58.43 | 0.008            | 18.91            | -                      |
| 418-1200 Eq. Baseline       | 40  | -13.7200 | -10.1285 | 1000.90    | 1008.44     | 56.17 | 0.008            | 18.98            | -                      |
| 418-1200 Eq. Baseline       | 41  | -13.7200 | -10.1475 | 1011.74    | 1008.03     | 53.93 | 0.008            | 19.06            | $T_{L}$                |
| 418-1200 Eq. Baseline       | 42  | -13.7200 | -10.1666 | 1022.33    | 1007.55     | 51.71 | 0.008            | 19.13            | $T_{\rm L}$            |
| 418-1200 Eq. Baseline       | 43  | -13.7200 | -10.1857 | 1032.69    | 1006.98     | 49.52 | 0.009            | 19.21            | $T_{\rm L}$            |
| 418-1200 Eq. Baseline       | 44  | -13.7200 | -10.2048 | 1042.83    | 1006.36     | 47.34 | 0.009            | 19.28            | $T_{\rm L}$            |
| 418-1200 Eq. Baseline       | 45  | -13.7200 | -10.2238 | 1052.74    | 1005.68     | 45.20 | 0.009            | 19.36            | $T_{\rm L}$            |
| 418-1200 Eq. Baseline       | 46  | -13.7200 | -10.2429 | 1062.45    | 1004.96     | 43.08 | 0.009            | 19.43            | $T_{ m L}$             |
| 418-1200 Eq. Baseline       | 47  | -13.7200 | -10.2620 | 1071.95    | 1004.19     | 41.00 | 0.009            | 19.51            | T <sub>L</sub>         |
| 418-1200 Eq. Baseline       | 48  | -13.7200 | -10.2811 | 1081.25    | 1003.40     | 38.94 | 0.010            | 19.58            | T <sub>L</sub>         |
| 418-1200 Eq. Baseline       | 49  | -13.7200 | -10.3002 | 1090.35    | 1002.58     | 36.92 | 0.010            | 19.65            | $T_{ m L}$             |

| Category                    | WL  | B ∆Gp    | B \( \Delta G p \) | $T_{ m L}$ | $T_{\rm L}$ | Visc  | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                    |
|-----------------------------|-----|----------|--------------------|------------|-------------|-------|------------------|------------------|------------------------|
|                             | (%) | MAR      | Value              | Pred       | MAR(°C)     | Pred  | wt%              | wt%              | Status                 |
|                             |     |          |                    | (°C)       |             | (P)   |                  |                  |                        |
| 418-1200 Eq. Baseline       | 50  | -13.7200 | -10.3192           | 1099.28    | 1001.73     | 34.93 | 0.010            | 19.73            | $T_{ m L}$             |
| 418-1200 Eq. Baseline       | 51  | -13.7200 | -10.3383           | 1108.01    | 1000.87     | 32.98 | 0.010            | 19.80            | $T_{ m L}$             |
| 418-1200 Eq. Baseline       | 52  | -13.7200 | -10.3574           | 1116.58    | 999.99      | 31.07 | 0.010            | 19.88            | $T_{ m L}$             |
| 418-1200 Eq. Baseline       | 53  | -13.7200 | -10.3765           | 1124.97    | 999.10      | 29.21 | 0.011            | 19.95            | $T_{ m L}$             |
| 418-1200 Eq. Baseline       | 54  | -13.7200 | -10.3955           | 1133.20    | 998.20      | 27.38 | 0.011            | 20.03            | $T_{ m L}$             |
| 418-1200 Eq. Baseline       | 55  | -13.7200 | -10.4146           | 1141.26    | 997.30      | 25.61 | 0.011            | 20.10            | $T_{ m L}$             |
| 418-1200 Eq. Baseline       | 56  | -13.7200 | -10.4337           | 1149.17    | 996.39      | 23.88 | 0.011            | 20.18            | $T_L$ , low $\eta$     |
| 418-1200 Eq. Baseline       | 57  | -13.7200 | -10.4528           | 1156.92    | 995.47      | 22.20 | 0.011            | 20.25            | T <sub>L</sub> , low η |
| 418-1200 Eq. Baseline       | 58  | -13.7200 | -10.4718           | 1164.53    | 994.55      | 20.57 | 0.012            | 20.33            | T <sub>L</sub> , low η |
| 418-1200 Eq. Baseline       | 59  | -13.7200 | -10.4909           | 1172.00    | 993.63      | 19.00 | 0.012            | 20.40            | $T_L$ , low $\eta$     |
| 418-1200 Eq. Baseline       | 60  | -13.7200 | -10.5100           | 1179.32    | 992.71      | 17.48 | 0.012            | 20.47            | T <sub>L</sub> , low η |
| 418-1200 Eq. Baseline w CST | 25  | -13.7200 | -9.7351            | 792.40     | 998.96      | 92.71 | 0.418            | 17.75            | -                      |
| 418-1200 Eq. Baseline w CST | 26  | -13.7200 | -9.7499            | 807.96     | 1001.10     | 90.36 | 0.435            | 17.82            | -                      |
| 418-1200 Eq. Baseline w CST | 27  | -13.7200 | -9.7647            | 823.09     | 1003.10     | 88.01 | 0.452            | 17.89            | -                      |
| 418-1200 Eq. Baseline w CST | 28  | -13.7200 | -9.7794            | 837.81     | 1004.49     | 85.67 | 0.468            | 17.96            | -                      |
| 418-1200 Eq. Baseline w CST | 29  | -13.7200 | -9.7942            | 852.15     | 1005.40     | 83.32 | 0.485            | 18.03            | -                      |
| 418-1200 Eq. Baseline w CST | 30  | -13.7200 | -9.8090            | 866.11     | 1006.25     | 80.99 | 0.502            | 18.10            | -                      |
| 418-1200 Eq. Baseline w CST | 31  | -13.7200 | -9.8238            | 879.72     | 1007.03     | 78.65 | 0.519            | 18.17            | -                      |
| 418-1200 Eq. Baseline w CST | 32  | -13.7200 | -9.8386            | 892.99     | 1007.73     | 76.33 | 0.535            | 18.24            | -                      |
| 418-1200 Eq. Baseline w CST | 33  | -13.7200 | -9.8534            | 905.93     | 1008.35     | 74.00 | 0.552            | 18.31            | -                      |
| 418-1200 Eq. Baseline w CST | 34  | -13.7200 | -9.8682            | 918.54     | 1008.86     | 71.69 | 0.569            | 18.38            | -                      |
| 418-1200 Eq. Baseline w CST | 35  | -13.7200 | -9.8830            | 930.86     | 1009.27     | 69.39 | 0.586            | 18.45            | -                      |
| 418-1200 Eq. Baseline w CST | 36  | -13.7200 | -9.8977            | 942.88     | 1009.57     | 67.10 | 0.602            | 18.52            | -                      |
| 418-1200 Eq. Baseline w CST | 37  | -13.7200 | -9.9125            | 954.61     | 1009.76     | 64.82 | 0.619            | 18.59            | -                      |
| 418-1200 Eq. Baseline w CST | 38  | -13.7200 | -9.9273            | 966.08     | 1009.83     | 62.55 | 0.636            | 18.66            | -                      |
| 418-1200 Eq. Baseline w CST | 39  | -13.7200 | -9.9421            | 977.28     | 1009.79     | 60.29 | 0.652            | 18.73            | -                      |
| 418-1200 Eq. Baseline w CST | 40  | -13.7200 | -9.9569            | 988.22     | 1009.65     | 58.05 | 0.669            | 18.80            | -                      |
| 418-1200 Eq. Baseline w CST | 41  | -13.7200 | -9.9717            | 998.92     | 1009.40     | 55.83 | 0.686            | 18.87            | -                      |
| 418-1200 Eq. Baseline w CST | 42  | -13.7200 | -9.9865            | 1009.38    | 1009.07     | 53.63 | 0.703            | 18.94            | $T_{ m L}$             |
| 418-1200 Eq. Baseline w CST | 43  | -13.7200 | -10.0013           | 1019.60    | 1008.65     | 51.44 | 0.719            | 19.01            | $T_{ m L}$             |
| 418-1200 Eq. Baseline w CST | 44  | -13.7200 | -10.0161           | 1029.61    | 1008.16     | 49.28 | 0.736            | 19.08            | $T_{ m L}$             |
| 418-1200 Eq. Baseline w CST | 45  | -13.7200 | -10.0308           | 1039.40    | 1007.61     | 47.14 | 0.753            | 19.15            | $T_{ m L}$             |

| Category                    | WL  | B ∆Gp    | B \( \Delta G p \) | $T_{ m L}$ | $T_{ m L}$ | Visc       | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                    |
|-----------------------------|-----|----------|--------------------|------------|------------|------------|------------------|------------------|------------------------|
| 9 ,                         | (%) | MAR      | Value              | Pred       | MAR(°C)    | Pred       | wt%              | wt%              | Status                 |
|                             |     |          |                    | (°C)       | , ,        | <b>(P)</b> |                  |                  |                        |
| 418-1200 Eq. Baseline w CST | 46  | -13.7200 | -10.0456           | 1048.98    | 1007.00    | 45.03      | 0.770            | 19.22            | $T_{\rm L}$            |
| 418-1200 Eq. Baseline w CST | 47  | -13.7200 | -10.0604           | 1058.35    | 1006.34    | 42.94      | 0.786            | 19.29            | $T_{ m L}$             |
| 418-1200 Eq. Baseline w CST | 48  | -13.7200 | -10.0752           | 1067.53    | 1005.65    | 40.88      | 0.803            | 19.36            | $T_{ m L}$             |
| 418-1200 Eq. Baseline w CST | 49  | -13.7200 | -10.0900           | 1076.52    | 1004.92    | 38.86      | 0.820            | 19.43            | $T_{ m L}$             |
| 418-1200 Eq. Baseline w CST | 50  | -13.7200 | -10.1048           | 1085.33    | 1004.16    | 36.86      | 0.837            | 19.50            | $T_{ m L}$             |
| 418-1200 Eq. Baseline w CST | 51  | -13.7200 | -10.1196           | 1093.95    | 1003.38    | 34.90      | 0.853            | 19.57            | $T_{ m L}$             |
| 418-1200 Eq. Baseline w CST | 52  | -13.7200 | -10.1344           | 1102.40    | 1002.58    | 32.97      | 0.870            | 19.64            | $T_{ m L}$             |
| 418-1200 Eq. Baseline w CST | 53  | -13.7200 | -10.1492           | 1110.68    | 1001.77    | 31.08      | 0.887            | 19.71            | $T_{ m L}$             |
| 418-1200 Eq. Baseline w CST | 54  | -13.7200 | -10.1639           | 1118.80    | 1000.94    | 29.24      | 0.903            | 19.78            | $T_{ m L}$             |
| 418-1200 Eq. Baseline w CST | 55  | -13.7200 | -10.1787           | 1126.76    | 1000.10    | 27.43      | 0.920            | 19.85            | $T_{ m L}$             |
| 418-1200 Eq. Baseline w CST | 56  | -13.7200 | -10.1935           | 1134.56    | 999.25     | 25.67      | 0.937            | 19.92            | $T_{ m L}$             |
| 418-1200 Eq. Baseline w CST | 57  | -13.7200 | -10.2083           | 1142.21    | 998.39     | 23.96      | 0.954            | 19.99            | $T_L$ , low $\eta$     |
| 418-1200 Eq. Baseline w CST | 58  | -13.7200 | -10.2231           | 1149.72    | 997.53     | 22.29      | 0.970            | 20.06            | T <sub>L</sub> , low η |
| 418-1200 Eq. Baseline w CST | 59  | -13.7200 | -10.2379           | 1157.08    | 996.67     | 20.68      | 0.987            | 20.13            | T <sub>L</sub> , low η |
| 418-1200 Eq. Baseline w CST | 60  | -13.7200 | -10.2527           | 1164.30    | 995.80     | 19.12      | 1.004            | 20.20            | T <sub>L</sub> , low η |
| 440-1200 Eq. Baseline       | 25  | -13.5866 | -14.8392           | 724.32     | 993.29     | 59.09      | 0.005            | 23.11            | $\Delta G_{P}$         |
| 440-1200 Eq. Baseline       | 26  | -13.5877 | -14.7916           | 739.99     | 995.24     | 57.41      | 0.005            | 23.12            | $\Delta G_{P}$         |
| 440-1200 Eq. Baseline       | 27  | -13.5887 | -14.7441           | 755.32     | 996.27     | 55.74      | 0.005            | 23.12            | $\Delta G_{P}$         |
| 440-1200 Eq. Baseline       | 28  | -13.5897 | -14.6965           | 770.31     | 997.29     | 54.07      | 0.006            | 23.13            | $\Delta G_{P}$         |
| 440-1200 Eq. Baseline       | 29  | -13.5907 | -14.6490           | 784.99     | 998.29     | 52.42      | 0.006            | 23.13            | $\Delta G_{P}$         |
| 440-1200 Eq. Baseline       | 30  | -13.5918 | -14.6014           | 799.37     | 999.27     | 50.77      | 0.006            | 23.14            | $\Delta G_{P}$         |
| 440-1200 Eq. Baseline       | 31  | -13.5928 | -14.5539           | 813.45     | 1000.22    | 49.13      | 0.006            | 23.14            | $\Delta G_{P}$         |
| 440-1200 Eq. Baseline       | 32  | -13.5938 | -14.5064           | 827.25     | 1001.14    | 47.50      | 0.006            | 23.15            | $\Delta G_{P}$         |
| 440-1200 Eq. Baseline       | 33  | -13.5948 | -14.4588           | 840.78     | 1002.03    | 45.87      | 0.007            | 23.15            | $\Delta G_{P}$         |
| 440-1200 Eq. Baseline       | 34  | -13.5958 | -14.4113           | 854.05     | 1002.87    | 44.27      | 0.007            | 23.16            | $\Delta G_{P}$         |
| 440-1200 Eq. Baseline       | 35  | -13.5968 | -14.3637           | 867.06     | 1003.67    | 42.67      | 0.007            | 23.16            | $\Delta G_{P}$         |
| 440-1200 Eq. Baseline       | 36  | -13.5977 | -14.3162           | 879.82     | 1004.40    | 41.09      | 0.007            | 23.16            | $\Delta G_{P}$         |
| 440-1200 Eq. Baseline       | 37  | -13.5987 | -14.2686           | 892.35     | 1005.08    | 39.52      | 0.007            | 23.17            | $\Delta G_{P}$         |
| 440-1200 Eq. Baseline       | 38  | -13.5997 | -14.2211           | 904.65     | 1005.68    | 37.96      | 0.008            | 23.17            | $\Delta G_{P}$         |
| 440-1200 Eq. Baseline       | 39  | -13.6006 | -14.1735           | 916.72     | 1006.21    | 36.43      | 0.008            | 23.18            | $\Delta G_{P}$         |
| 440-1200 Eq. Baseline       | 40  | -13.6016 | -14.1260           | 928.58     | 1006.65    | 34.91      | 0.008            | 23.18            | $\Delta G_{P}$         |
| 440-1200 Eq. Baseline       | 41  | -13.6025 | -14.0784           | 940.23     | 1007.00    | 33.40      | 0.008            | 23.19            | $\Delta G_{P}$         |

| Category                    | WL  | B ΔGp    | B \( \Delta G p \) | $T_{ m L}$ | $T_{\rm L}$ | Visc  | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                        |
|-----------------------------|-----|----------|--------------------|------------|-------------|-------|------------------|------------------|----------------------------|
|                             | (%) | MAR      | Value              | Pred       | MAR(°C)     | Pred  | wt%              | wt%              | Status                     |
|                             |     |          |                    | (°C)       |             | (P)   |                  |                  |                            |
| 440-1200 Eq. Baseline       | 42  | -13.6035 | -14.0309           | 951.67     | 1007.25     | 31.92 | 0.008            | 23.19            | $\Delta G_{P}$             |
| 440-1200 Eq. Baseline       | 43  | -13.6044 | -13.9833           | 962.91     | 1007.40     | 30.46 | 0.009            | 23.20            | $\Delta G_{P}$             |
| 440-1200 Eq. Baseline       | 44  | -13.6053 | -13.9358           | 973.96     | 1007.46     | 29.02 | 0.009            | 23.20            | $\Delta G_{P}$             |
| 440-1200 Eq. Baseline       | 45  | -13.6063 | -13.8882           | 984.82     | 1007.41     | 27.60 | 0.009            | 23.21            | $\Delta G_{P}$             |
| 440-1200 Eq. Baseline       | 46  | -13.6072 | -13.8407           | 995.50     | 1007.26     | 26.20 | 0.009            | 23.21            | $\Delta G_{P}$             |
| 440-1200 Eq. Baseline       | 47  | -13.6081 | -13.7931           | 1006.00    | 1007.03     | 24.84 | 0.009            | 23.22            | $\Delta G_{P}$             |
| 440-1200 Eq. Baseline       | 48  | -13.6090 | -13.7456           | 1016.32    | 1006.70     | 23.49 | 0.010            | 23.22            | $\Delta G_P$ , $T_L$ , low |
|                             |     |          |                    |            |             |       |                  |                  | η                          |
| 440-1200 Eq. Baseline       | 49  | -13.6099 | -13.6980           | 1026.48    | 1006.30     | 22.18 | 0.010            | 23.22            | $\Delta G_P$ , $T_L$ , low |
|                             |     |          |                    |            |             |       |                  |                  | η                          |
| 440-1200 Eq. Baseline       | 50  | -13.6108 | -13.6505           | 1036.47    | 1005.82     | 20.89 | 0.010            | 23.23            | $\Delta G_P$ , $T_L$ , low |
|                             |     |          |                    |            |             |       |                  |                  | η                          |
| 440-1200 Eq. Baseline       | 51  | -13.6116 | -13.6029           | 1046.31    | 1005.28     | 19.64 | 0.010            | 23.23            | $\Delta G_P, T_L, low$     |
|                             |     |          |                    |            |             |       |                  |                  | η                          |
| 440-1200 Eq. Baseline       | 52  | -13.6125 | -13.5554           | 1055.98    | 1004.68     | 18.42 | 0.010            | 23.24            | $\Delta G_P$ , $T_L$ , low |
|                             |     |          |                    |            |             |       |                  |                  | η                          |
| 440-1200 Eq. Baseline       | 53  | -13.6134 | -13.5078           | 1065.50    | 1004.02     | 17.22 | 0.011            | 23.24            | $\Delta G_P$ , $T_L$ , low |
|                             |     |          |                    |            |             |       |                  |                  | η                          |
| 440-1200 Eq. Baseline       | 54  | -13.6142 | -13.4603           | 1074.88    | 1003.32     | 16.07 | 0.011            | 23.25            | $\Delta G_P$ , $T_L$ , low |
|                             |     |          |                    |            |             |       |                  |                  | η                          |
| 440-1200 Eq. Baseline       | 55  | -13.6151 | -13.4128           | 1084.11    | 1002.58     | 14.95 | 0.011            | 23.25            | $\Delta G_P, T_L, low$     |
|                             |     |          |                    |            |             |       |                  |                  | η                          |
| 440-1200 Eq. Baseline       | 56  | -13.6159 | -13.3652           | 1093.19    | 1001.80     | 13.86 | 0.011            | 23.26            | $T_L$ , low $\eta$         |
| 440-1200 Eq. Baseline       | 57  | -13.6168 | -13.3177           | 1102.14    | 1000.99     | 12.81 | 0.011            | 23.26            | $T_L$ , low $\eta$         |
| 440-1200 Eq. Baseline       | 58  | -13.6176 | -13.2701           | 1110.95    | 1000.16     | 11.81 | 0.012            | 23.27            | $T_L$ , low $\eta$         |
| 440-1200 Eq. Baseline       | 59  | -13.6184 | -13.2226           | 1119.63    | 999.30      | 10.84 | 0.012            | 23.27            | $T_L$ , low $\eta$         |
| 440-1200 Eq. Baseline       | 60  | -13.6193 | -13.1750           | 1128.18    | 998.42      | 9.91  | 0.012            | 23.27            | $T_L$ , low $\eta$         |
| 440-1200 Eq. Baseline w CST | 25  | -13.5895 | -14.7320           | 714.68     | 991.80      | 60.17 | 0.418            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 26  | -13.5906 | -14.6801           | 730.13     | 993.99      | 58.52 | 0.435            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 27  | -13.5918 | -14.6283           | 745.24     | 995.87      | 56.88 | 0.452            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 28  | -13.5929 | -14.5765           | 760.03     | 996.85      | 55.25 | 0.468            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 29  | -13.5941 | -14.5246           | 774.51     | 997.82      | 53.62 | 0.485            | 23.00            | $\Delta G_{P}$             |

| Category                    | WL  | B ∆Gp    | B ∆Gp    | $T_{ m L}$ | $T_{ m L}$ | Visc       | TiO <sub>2</sub> | R <sub>2</sub> O | MAR                        |
|-----------------------------|-----|----------|----------|------------|------------|------------|------------------|------------------|----------------------------|
|                             | (%) | MAR      | Value    | Pred       | MAR(°C)    | Pred       | wt%              | wt%              | Status                     |
|                             |     |          |          | (°C)       | , ,        | <b>(P)</b> |                  |                  |                            |
| 440-1200 Eq. Baseline w CST | 30  | -13.5952 | -14.4728 | 788.69     | 998.78     | 52.00      | 0.502            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 31  | -13.5963 | -14.4209 | 802.59     | 999.71     | 50.38      | 0.519            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 32  | -13.5975 | -14.3691 | 816.20     | 1000.63    | 48.78      | 0.535            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 33  | -13.5986 | -14.3173 | 829.55     | 1001.51    | 47.18      | 0.552            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 34  | -13.5997 | -14.2654 | 842.64     | 1002.35    | 45.59      | 0.569            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 35  | -13.6008 | -14.2136 | 855.48     | 1003.16    | 44.02      | 0.586            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 36  | -13.6019 | -14.1618 | 868.08     | 1003.92    | 42.45      | 0.602            | 23.00            | $\Delta G_{P}$             |
| 440-1200 Eq. Baseline w CST | 37  | -13.6030 | -14.1099 | 880.44     | 1004.63    | 40.90      | 0.619            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 38  | -13.6041 | -14.0581 | 892.58     | 1005.29    | 39.36      | 0.636            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 39  | -13.6051 | -14.0063 | 904.50     | 1005.88    | 37.83      | 0.652            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 40  | -13.6062 | -13.9544 | 916.20     | 1006.39    | 36.32      | 0.669            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 41  | -13.6073 | -13.9026 | 927.70     | 1006.84    | 34.83      | 0.686            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 42  | -13.6083 | -13.8507 | 938.99     | 1007.20    | 33.35      | 0.703            | 23.00            | $\Delta G_{P}$             |
| 440-1200 Eq. Baseline w CST | 43  | -13.6094 | -13.7989 | 950.09     | 1007.48    | 31.89      | 0.719            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 44  | -13.6104 | -13.7471 | 961.00     | 1007.66    | 30.45      | 0.736            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 45  | -13.6115 | -13.6952 | 971.72     | 1007.76    | 29.03      | 0.753            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 46  | -13.6125 | -13.6434 | 982.26     | 1007.77    | 27.63      | 0.770            | 23.00            | $\Delta G_{P}$             |
| 440-1200 Eq. Baseline w CST | 47  | -13.6135 | -13.5916 | 992.63     | 1007.68    | 26.26      | 0.786            | 23.00            | $\Delta G_{ m P}$          |
| 440-1200 Eq. Baseline w CST | 48  | -13.6145 | -13.5397 | 1002.82    | 1007.51    | 24.91      | 0.803            | 23.00            | $\Delta G_{P}$             |
| 440-1200 Eq. Baseline w CST | 49  | -13.6156 | -13.4879 | 1012.85    | 1007.26    | 23.59      | 0.820            | 23.00            | $\Delta G_P$ , $T_L$ , low |
|                             |     |          |          |            |            |            |                  |                  | η                          |
| 440-1200 Eq. Baseline w CST | 50  | -13.6166 | -13.4361 | 1022.72    | 1006.94    | 22.29      | 0.837            | 23.00            | $\Delta G_P$ , $T_L$ , low |
|                             |     |          |          |            |            |            |                  |                  | η                          |
| 440-1200 Eq. Baseline w CST | 51  | -13.6176 | -13.3842 | 1032.43    | 1006.54    | 21.02      | 0.853            | 23.00            | $\Delta G_P$ , $T_L$ , low |
|                             |     |          |          |            |            |            |                  |                  | η                          |
| 440-1200 Eq. Baseline w CST | 52  | -13.6185 | -13.3324 | 1041.98    | 1006.07    | 19.77      | 0.870            | 23.00            | $T_L$ , low $\eta$         |
| 440-1200 Eq. Baseline w CST | 53  | -13.6195 | -13.2805 | 1051.38    | 1005.55    | 18.56      | 0.887            | 23.00            | $T_L$ , low $\eta$         |
| 440-1200 Eq. Baseline w CST | 54  | -13.6205 | -13.2287 | 1060.64    | 1004.98    | 17.38      | 0.903            | 23.00            | $T_L$ , low $\eta$         |
| 440-1200 Eq. Baseline w CST | 55  | -13.6215 | -13.1769 | 1069.75    | 1004.36    | 16.23      | 0.920            | 23.00            | $T_L$ , low $\eta$         |
| 440-1200 Eq. Baseline w CST | 56  | -13.6224 | -13.1250 | 1078.72    | 1003.69    | 15.12      | 0.937            | 23.00            | $T_L$ , low $\eta$         |
| 440-1200 Eq. Baseline w CST | 57  | -13.6234 | -13.0732 | 1087.56    | 1002.99    | 14.04      | 0.954            | 23.00            | $T_L$ , low $\eta$         |
| 440-1200 Eq. Baseline w CST | 58  | -13.6243 | -13.0214 | 1096.26    | 1002.26    | 13.00      | 0.970            | 23.00            | $T_L$ , low $\eta$         |

| Category                    | WL<br>(%) | B ∆Gp<br>MAR | B ∆Gp<br>Value | T <sub>L</sub><br>Pred | T <sub>L</sub><br>MAR(°C) | Visc<br>Pred | TiO <sub>2</sub> wt% | R <sub>2</sub> O<br>wt% | MAR<br>Status      |
|-----------------------------|-----------|--------------|----------------|------------------------|---------------------------|--------------|----------------------|-------------------------|--------------------|
|                             |           |              |                | (°C)                   |                           | <b>(P)</b>   |                      |                         |                    |
| 440-1200 Eq. Baseline w CST | 59        | -13.6253     | -12.9695       | 1104.83                | 1001.50                   | 11.99        | 0.987                | 23.00                   | $T_L$ , low $\eta$ |
| 440-1200 Eq. Baseline w CST | 60        | -13.6262     | -12.9177       | 1113.27                | 1000.71                   | 11.03        | 1.004                | 23.00                   | $T_L$ , low $\eta$ |

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| Distribution:  |                   |                                  |                            |                |                |                                       |                            |  |
|----------------|-------------------|----------------------------------|----------------------------|----------------|----------------|---------------------------------------|----------------------------|--|
| R. A.          | Adams             | 241-162H, Rm. 4                  | (E)                        | T. J.          | Lex            | 703-H, Rm. 16                         | <b>(E)</b>                 |  |
| K. A.<br>J. W. | Barber            |                                  | (E)<br>(E)                 | 1. J.<br>D. B. | Little         | 703-H, Rm. 3                          | (E)                        |  |
| J. W.<br>J. L. |                   | 704-2H, Rm. 197                  |                            | D. B.<br>S. R. | Loflin         | · · · · · · · · · · · · · · · · · · · | (E)                        |  |
|                | Barnes            | 704-S, Rm. 19                    | (E)                        |                |                | 773-41A, Rm. 223                      | (E)                        |  |
| M. J.          | Barnes            | 773-A, Rm. B-132                 | (E)                        | N. P.          | Malik          | 704-26F, Rm. 11                       | (E)                        |  |
| W. M.          | Barnes            | 704-56H, Rm. 164                 | (E)                        | J. C.          | Marra          | 773-42A, Rm. 173                      | (E)                        |  |
| S. M.          | Blanco            | 766-H. Rm. 2434                  | (E)                        | D. J.          | Martin         | 742-4G, Rm. 5                         | (E)                        |  |
| L. R.          | Bragg             | 766-H, Rm. 2434                  | (E)                        | K. B.          | Martin         | 773-42A, Rm. 14                       | (E)                        |  |
| T. E.          | Britt             | 742-4G, Rm. 3                    | (E)                        | C. J.          | Martino        | 735-11A, Rm. 121                      | (E)                        |  |
| H. L.          | Bui               | 742-4G, Rm. 3                    | (E)                        | G. A.          | Mathis         | 724-9E, Rm. 1                         | (E)                        |  |
| S. G.          | Campbell          | 703-H, Rm. 107                   | (E)                        | G. J.          | Matis          | 766-H, Rm. 1066F                      | (E)                        |  |
| L.             | Carey             | 766-H, Rm. 2005A                 | (E)                        | D.             | Maxwell        | 766-H, Rm. 2231                       | (E)                        |  |
| J. T.          | Carter            | 703-H, Rm 122                    | (E)                        | J. W.          | McCullough     | 766-H, Rm. 2411                       | (E)                        |  |
| W. D.          | Clark             | 766-H, Rm. 2412                  | (E)                        | L. T.          | McGuire        | 766-H, Rm. 2441                       | (E)                        |  |
| S. L.          | Clifford          | 766-H, Rm. 2443                  | (E)                        | C. A.          | Nash           | 773-42A, Rm. 182                      | (E)                        |  |
| J. J.          | Connelly          | 773-41A, Rm. 231                 | (E)                        | L. M.          | Nelson         | 773-43A, Rm. 222                      | (E)                        |  |
| D. T.          | Conrad            | 766-H, Rm. 2007                  | (E)                        | M. A.          | Norato         | 704-27S, Rm. 6                        | (E)                        |  |
| D. R.          | Cox               | 730-2B, Rm. 118                  | (E)                        | M. R.          | Norton         | 766-H, Rm. 2002                       | (E)                        |  |
| A. D.          | Cozzi             | 773-43A, Rm. 218                 | (E)                        | J. E.          | Occhipinti     | 704-S, Rm. 18                         | <b>(E)</b>                 |  |
| C. L.          | Crawford          | 773-41A, Rm. 180                 | (E)                        | L. D.          | Olson          | 703-H, Rm. 5                          | <b>(E)</b>                 |  |
| D. A.          | Crowley           | 773-A, Rm. A-262                 | (E)                        | T. L.          | Ortner         | 766-H, Rm. 2009                       | <b>(E)</b>                 |  |
| N. R.          | Davis             | 766-H, Rm. 1006                  | (E)                        |                | _              |                                       |                            |  |
| W. B.          | Dean              | 766-H, Rm. 2243                  | (E)                        | T. B.          | Peters         | 773-42A, Rm. 128                      | <b>(E)</b>                 |  |
| V. G.          | Dickert           | 703-H, Rm. 4                     | <b>(E)</b>                 | J. A.          | Pike           | 703-H, Rm. 99                         | <b>(E)</b>                 |  |
| C. L.          | Donahue           | 241-162H, Rm. 6                  | <b>(E)</b>                 | M. R.          | Poirier        | 773-42A, Rm. 123                      | <b>(E)</b>                 |  |
| M. D.          | Drumm             | 766-H, Rm. 2050                  | <b>(E)</b>                 | S. H.          | Reboul         | 703-H, Rm. 84                         | <b>(E)</b>                 |  |
| M. C.          | Duff              | 773-43A, Rm. 217                 | <b>(E)</b>                 | T. R.          | Reynolds       | 704-S, Rm. 65                         | <b>(E)</b>                 |  |
| C. R.          | Dyer              | 766-H, Rm. 2426                  | <b>(E)</b>                 | M. A.          | Rios-Armstrong | 766-H, Rm 2054                        | <b>(E)</b>                 |  |
| R. E.          | Eibling           | 999-W, Rm. 335                   | (E)                        | S. J.          | Robertson      | 766-H, Rm. 2500                       | (P)                        |  |
| G. N.          | Eide              | 241-121H, Rm. 6                  | (E)                        | B. C.          | Rogers         | 766-H, Rm. 2008                       | <b>(E)</b>                 |  |
| Н. Н.          | Elder             | 703-H, Rm. 95                    | (E)                        | R. A.          | Runnels        | 766-H, Rm. 2011                       | <b>(E)</b>                 |  |
| S. D.          | Fink              | 773-A, Rm. B-112                 | $(\mathbf{E}, \mathbf{P})$ | P. J.          | Ryan           | 704-61S, Rm. 6                        | <b>(E)</b>                 |  |
| F. F.          | Fondeur           | 773-A, Rm. B-124                 | (E)                        | E.             | Saldivar       | 766-H, Rm. 2004                       | <b>(E)</b>                 |  |
| R. C.          | Fowler            | 703-H, Rm. 98                    | (E)                        | S. C.          | Shah           | 766-H, Rm. 2037                       | <b>(E)</b>                 |  |
| M.W.           | Geeting           | 766-H, Rm. 2035                  | (E)                        | T. J.          | Spears         | 766-H, Rm. 2015                       | (E)                        |  |
| B. A.          | Gifford           | 766-H, Rm. 1066D                 | (E)                        | R. H.          | Spires         | 766-H, Rm. 2003                       | (E)                        |  |
| A. P.          | Giordano          | 703-H, Rm 79                     | (E)                        | M. E.          | Stallings      | 773-A, Rm. B-117                      | (E)                        |  |
| J. C.          | Griffin           | 773-A, rm. A-231                 | (E)                        | W. E.          | Stevens        | 773-A, Rm. A-261                      | (E)                        |  |
| H. D.          | Harmon            | 766-H, Rm. 2014                  | (P)                        | S. J.          | Strohmeier     | 766-H, Rm. 2022                       | (E)                        |  |
| K. D.          | Harp              | 755-H, Rm. 1066B                 | (E)                        | S. G.          | Subosits       | 766-H, Rm. 2052                       | (E)                        |  |
| E. W.          | Harrison          | 766-H, Rm. 2034                  | (E)                        | P. C.          | Suggs          | 766-H, Rm. 2436                       | (E)                        |  |
| K. A.          | Hauer             | 703-H, Rm. 11                    | (E)                        | G. A.          | Taylor         | 703-H, Rm. 96                         | (E)                        |  |
| D. T.          | Herman            | 735-11A, Rm. 104                 | (E)                        | S. A.          | Thomas         | 766-H, Rm. 2016                       | (E)                        |  |
| R. N.          | Hinds             | 766-H, Rm. 2430                  | (E)                        | P. J.          | Valenti        | 730-4B, Rm. 2062                      | (E)                        |  |
| D. T.          | Hobbs             | 773-A, Rm. B-117                 | (E)                        | W.B.           | Van-Pelt       | 704-S, Rm. 16                         | (E)                        |  |
| E. W.          | Holtzscheiter     | 773-A, Rm. A-230                 | (E)                        | D. D.          | Walker         | 773-A, Rm. B-124                      | (E)                        |  |
| C. M.          | Jantzen           | 773-A, Rm. B-104                 | (E)                        | A. O.          | Waring         | 766-H, Rm. 2423                       | (E)                        |  |
| R. T.          | Jones             | 766-H, Rm. 2463                  | (E)                        | F. A.          | Washburn       | 766-H, Rm. 2054                       | (E)                        |  |
| W. D.          | Kerley            | 766-H, Rm. 2010                  | (E)                        | V.B.           | Wheeler        | 766-H, Rm. 2438                       | (E)                        |  |
| E. T.          | Ketusky           | 703-H, Rm. 83                    | (E)                        | G. G.          | Wicks          | 773-A, Rm. B-129                      | (E)                        |  |
| D. P.          | Lambert           | 773-A, Rm. B-132                 | (E)                        | W. R.          | Wilmarth       | 773-42A, Rm. 171                      | (E)                        |  |
| C. A.          | Lanigan           | 766-H, Rm. 2440B                 | (E)                        | G. C.          | Winship        | 766-H, Rm. 2024                       | (E)                        |  |
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